Partners for Innovation

FIRST DRAFT OF CASE STUDY 1.1: DETERGENT BOTTLE

An example of weighing sustainability criteria for rigid plastic non-food packaging

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CONTENT

1. INTRODUCTION

Global plastics production has reached 311 million metric tons and is expected to continue to grow by around 4% annually for the foreseeable future. While plastics deliver many benefits to society, there is an increasing awareness of the potential impact of chemical components of plastics on human health and the environment.

The Organisation for Economic Co-operation and Development (OECD) organised a Global Forum on Environment focussed on "Plastics in a Circular Economy: Design of Sustainable Plastics from a Chemicals Perspective" in 2018. The Forum sought to incentivise a shift in sustainable chemistry thinking at the product design stage by identifying good practices, including tools and approaches, as well as a policy framework to reduce the environmental and health plastics impacts. This resulted in multiple reports on the sustainability of plastics from a chemical perspective.

To build on this research and translate it to practical insights for packaging designers the OECD Global Forum for the Environment commissioned the development of this case study on sustainability criteria for plastic design for detergent bottles. In this case study a lifecycle approach is taken for the development of plastics for detergent bottles. All sustainability aspects regarding human health and the environment are considered, resulting in sustainability criteria that support decisions on sustainability for people throughout the value chain who are involved in the design of detergent bottles. This enables sustainable designs tailored to the specific life cycle scenario of a detergent bottle.

Another case study that is developed regards the sustainable design of plastics packaging film for biscuits. The two case studies conducted are intended to set an example for other sectors and product categories.

1.1 READING GUIDE

Life cycle approach

The sustainability criteria are assessed for the life cycle stages through which a detergent bottle cycles: sourcing of the material, production and filling of the bottle, using of the bottle and detergent, and end of use at which the bottle is discarded and processed. At each stage in the life cycle different considerations regarding sustainability come into play, while decisions in one stage might also affect the impact at other stages. From a designers' perspective this journey will start with the use phase. The purpose of the product and the context in which it will be used, determine the basic set of technical requirements and constraints for a shortlist of possible materials. Therefore this case study will consider the use phase first, after which the sourcing of the feedstock, the production of bottles and its end-of-use are discussed.

Case study structure

In the subsequent chapters the different life cycle stages will be discussed. Per chapter a general overview of the life cycle stage is provided, describing the different processes and relevant factors that influence sustainability of the packaging. The relevant sustainability factors are identified by keeping a list of Sustainable Design Goals in mind while working through the life cycle stages.

Each sustainability factor leads to key considerations; a decision that needs to be made to select a polymer or a chemical in the production of plastic detergent bottles. Polymer considerations describe what must be taken into account when selecting a polymer. Chemical considerations describe the subsequent choices that must be made in regard of chemical additives used in the production of detergent bottles, once a polymer has been selected.

Once all aspects of the life cycle have been considered, an overview of the key considerations and trade-offs is provided in Chapter 7. Subsequently, the different sustainability criteria emerging from the life cycle stages will be simultaneously assessed in the Material Assessment in Chapter 8.

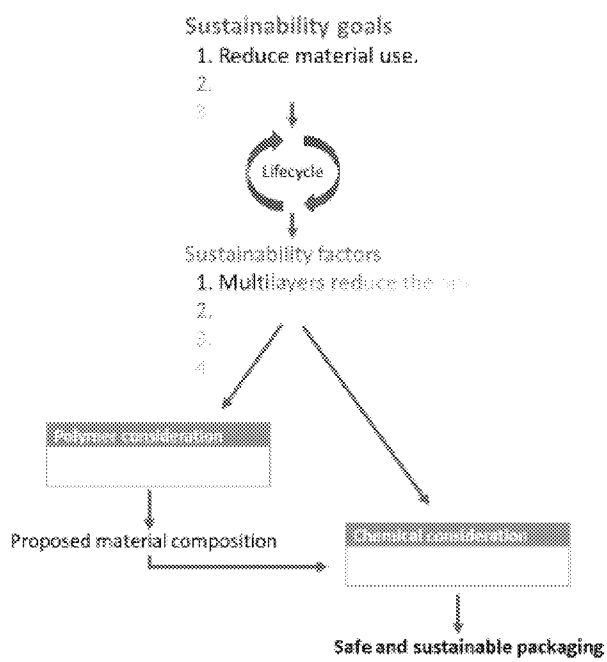

Figure 1-1

1.2 SCOPE

This case study investigates sustainability aspects of a rigid plastic packaging for laundry detergents. A detergent bottle typically consists of the following elements:

- **Bottle:** Rigid plastic bottle. Commonly made from HDPE, PP or PET polymers. Some bottles contain a handle for extra grip. In the market transparent bottles and a wide variety of colours can be found.
- **Closure:** Cap or spray nozzle that closes the bottle and can support dosing of the product.
- **Label:** Bottles contain labels that communicate necessary information to consumers and support marketing of the product. In the detergent isle wrap sleeves and traditional labels can be found.

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Figure 1-2: *Variation of (laundry) detergent bottles.*
Left to right: HDPE bottle, recycled PET bottle, PP bottle

Scope: Focus on bottle

This case study focusses on the rigid plastic detergent bottle. The closure and label are only considered when they influence the sustainability of bottle, e.g. in recycling. Closures and labels are not considered as separate entities in this case study and are therefore not investigated on a chemical level.

Case study relevance

Additionally, this case study will assess to what extend sustainability criteria from laundry detergent bottles are relevant and applicable to other detergent bottles, such as all-purpose cleaner, shampoo and soap bottles.

Out of scope

The following types of detergent packaging is out of scope:

- **(Refill) packaging multilayer films:** In the detergent aisle packaging multilayer films are increasingly seen as refill packaging or 'bag-in-box' packaging. In these multilayers different materials are laminated together into a film to obtain the preferred barrier properties. Subsequently, this film is used to produce a pouch. This type of packaging is out of scope as this case study is limited to rigid plastics.

1.3 SUSTAINABLE DESIGN GOALS

To guide the material and chemical selection, overarching sustainability goals need to be set. Using secondary feedstock for the production of bottles contributes to closing the material loop, but might require the use of more plastics. A chemical additive might increase efficiency in the production of the packaging and thus reduce the overall CO_2 emissions in the process, but it could hinder the recycling of the material at the end of use. Establishing overarching sustainability goals on forehand will enable the designer to look for these kinds of benefits and drawbacks when examining material alternatives. Furthermore, the goals will guide the designer in the selection of materials when trade-offs need to be made.

1. Prevent product spoilage

The packaging serves to protect the product. Usually the (environmental) impact of the product's production is far greater than that of the packaging's total lifecycle. Preventing spoilage of the product before it reaches its intended goal is an important goal in the sustainable design of the packaging.

For detergents product spoilage can be realised by preserving the product to prevent degradation of quality, and supporting the consumer in dosing the product.

2. Reduce material use

Packaging is a short-lived product, but amounts to 40% of the world's total use of plastic. Designers should strive to reduce the use of plastic to the absolute minimum to perform the packaging duties. In addition to light weighting material use can be reduced through reusable packaging.

3. Close material loops

Due to the short-lived use of packaging, the used material should make multiple lifecycles. The plastic should either be made from secondary feedstock or be able to be used a second time in another product. In an ideal situation a combination of both is made.

4. Preserve natural capital

Humans depend on natural capital for a wide range of ecosystem services. Poorly managed natural capital can destroy productivity and resilience, making it difficult for humans and other species to sustain themselves. Throughout its lifecycle the negative effects of the packaging on natural capital should be limited. This includes the chosen feedstock, but also includes effects of production and waste management at the end of life.

5. Guard health of participants in lifecycle

From feedstock extraction, through packaging manufacturing and product use to the eventual end-of-life scenario, the packaging and its subcomponents will interact with humans. The direct negative effects of the packaging and its subcomponents on the health of these people needs to minimized.

Examples of other sustainable design goals

The five goals listed above are chosen for this case study. Other sustainable design goals might be:

- Minimize waste
- Improve social conditions throughout the life cycle
- Decouple from fossil resources

1.4 DECISION MAKING PROCESS

During the design process the listed five sustainable design goals will be considered to select the most sustainable plastic(s) to be used in the packaging of laundry detergent. During the analysis of the lifecycle it will show that trade-offs will need to be made. The decision for one material based on one goal in one phase of the lifecycle will counteract the realisation of another goal in another part of the lifecycle. To be able to make the best overall decision the Hybrid Methodology will be used, combining sequential and simultaneous decision making.

Based on the overarching five sustainable design goals, sustainability considerations are identified. A polymer shortlist is created by evaluating the different polymer options on the key sustainability considerations. A final polymer selection should be made based the required technical specifications for the bottle on the local situation for which the packaging is designed. Subsequently, the polymer must be evaluated using the list of chemical considerations (Section 8.2). Finally, the bottle design should be carefully considered as this is an important factor in realising the sustainable design goals. The described decision making process should lead to a selection of polymer and additives that is the best fit for the detergent bottle to be designed.

2. ANALYSIS OF THE LIFE CYCLE

2.1 VISUAL OVERVIEW OF THE LIFECYCLE

Sourcing | Production | Use | End of use

Polymer resin producer
- Turns feedstock in polymer
- **End:** plain polymer granules

Compounder
- Mixes polymers to specifications of bottle producer
- **End:** polymer mixed with additives

Bottle producer
- Produces preforms and/or blows bottles
- **End:** Blown bottle

Detergent producer
- Uses bottle to pack detergent
- **End:** Bottle filled with detergent

Retailer
- Stores and sells detergent in bottle

User
- Uses detergent
- Disposes of bottle
- **End:** Packaging waste

Packaging waste sorter
- Bottle is sorted for recycling or becomes waste
- **End:** (un)sorted bottle

Material recycler
- Bottle is remelted to granules
- **End:** Recycled plastics granules

2.2 OVERVIEW OF SUSTAINABILITY IN THE LIFE CYCLE

In the table below an overview of the important sustainability factors per life cycle stage of a detergent bottle can be found, it is also indicated which sustainable design goals are relevant.

Table 2-1: Overview life cycle stages

	Sourcing of materials	Production	Use phase	End of use
	Production of polymer resin	Production, filling, labelling and closing of detergent bottle	Transportation to user, preservation and dosing of detergent	Disposal, sorting and recycling of detergent bottle
Important sustainability factors	- Polymer options for packaging - Polymer feedstock - Additives required for polymerisation - Safety of workers	- Production methods - Additives required in production of packaging - Additional chemicals used in production (non-ingredients) - Safety of workers	- Requirements for use (and transport) - Migration of packaging into detergent - Exposure information - Waste and pollution generated during product use	- End of use scenarios - Recyclability of design - Recyclability of polymers - Recyclability of additives - Safety of workers
Sustainable design goals	- Close material loops - Preserve natural capital - Guard the safety of participants in life cycle	- Prevent product spoilage - Reduce material use - Guard the safety of production workers	- Prevent product spoilage - Preserve natural capital - Guard the safety of consumers	- Close material loops - Preserve natural capital - Guard the safety of production workers

2.3 REGULATIONS ON CHEMICALS IN PLASTICS

Multiple national and international authorities have their own lists of substances that are prohibited or are limited in use for plastics.

EU: REACH

Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) is a regulation from the European Union to control the health and environmental risks of chemicals. It restricts the use of chemicals with known risks, oblige producers to communicate about the risks, and forces producers to register new chemicals and evaluate their risk to the environment and human health. Based on the hazard categories (discussed in paragraph 2.5) and the hazard level, substances are either banned or restricted in use.

Restricted Substances List of the Cradle to Cradle Products Innovation Institute

The Cradle to Cradle Products Innovation Institute is not a regulatory body that can restrict the use of substances in products in a given market. It is a non-profit organization that maintains a standard for products and materials to become 'Cradle to Cradle certified'. This is a certification for sustainable products and certifies them as safe, responsible, and fit for a circular economy. The Restricted Substances List (RSL) is a checklist for materials that cannot be used in certified products. The list is comprised of restrictions on chemicals from multiple existing chemical regulations such as the one mentioned above. The most conservative thresholds for each substance in any of the combined regulations is chosen. The fourth version of the RSL is expected in January 2021 and will be updated annually.

2.4 HAZARD CATEGORIES

In this paragraph the main hazard categories for human health will be discussed. To these categories will be referred when discussing chemicals in the lifecycle phases. The chemicals can pose risks in all lifecycle phases: to a consumer when he interacts with the packaging, but also to a plant operator in the production of the packaging, or to recycling facility staff or life in the nearby environment at the End of Use phase. These categories are the ones defined under the EU's REACH regulation.

CMR

This category contains substances that are

- Carcinogenic: causes cancer growth
- Mutagenic: alters genetic material or increases mutations
- Reprotoxic: causes infertility or reduces development of offspring

PBT and vPvB

Two other categories defined in REACH regulation. PBT are substances that are:

- Persistent: do not degrade or degrade very slowly in the environment or in organisms
- Bioaccumulative: accumulate in organisms faster than they are excreted or degraded
- Toxic: causes harm when inhaled, ingested, absorbed, or touched

vPvB stands for very Persistent or very Bioaccumulative.

Endocrine disrupting chemicals (EDC)

Substances that interfere with the regular functioning of hormones and hormone receptors

2.5 INCORPORATION OF SAFE CHEMICAL SELECTION IN THE DESIGN PROCESS

With this document the following method for selection of chemicals for detergent bottles is proposed:

1. Demand from all your suppliers that they adhere to the local regulations for safe materials.
2. Use a lifecycle approach to map out the relevant considerations concerning chemicals and their effects throughout all lifecycle stages.
3. Select a material for the packaging according to the decision-making process, explained on in Section 8.1.
4. Check, in collaboration with your material supplier if necessary, whether the found chemical considerations involve any of the substances on the Restricted Substances List (RSL) of the Cradle to Cradle Products Innovation Institute.
5. If substances on the RSL are part of a chemical consideration, try to find an alternative substance for the intended goal.

6. If no alternative is possible, verify that the concentration of the substance is below the limit set in the RSL.
7. If incorporation of substances on the RSL is inevitable for the product, verify through relevant migration tests that these substances do not pose a hazard in the bottle lifecycle.
8. If steps 6 or 7 cannot be passed, revisit step 3 and select another material or material combination.

3. USE PHASE

This phase touches upon three of the overarching sustainability goals:

1. **Prevent product spoilage:** Preserve the washing detergent during transport and use period (shelf life) and support correct dosing of the detergent to prevent product spoilage.
2. **Preserve natural capital:** Prevent leakage of chemicals to the environment e.g. with waste water form washing into the waste water system. Limit green house emissions caused by transport of the filled packaging.
3. **Guard the safety of consumers:** Prevent exposure of humans to hazardous chemicals in the packaging during use, and prevent migration of hazardous chemicals into the detergent which might subsequently adhere to washed clothing and thereupon come in contact with the user's skin.

3.1 FUNCTIONAL REQUIREMENTS AND BOTTLE DESIGN

In the use phase the packaging is used for its intended goal: safely transporting the detergent from the producer to the consumer, attracting attention of consumers in the store, providing information to the consumer, preserving the liquid and support its dosing. Below the required packaging functionalities that influence the sustainable design goals of *Product spoilage* and *Preservation of natural capital* (through efficient transport) are addressed.

Transport detergent to consumer

Strength and stiffness: One of the primary functionalities of a detergent bottle is containing the liquid detergent and transporting it safely from the production site, to the retailer and finally the consumer. A bottle must thus provide sufficient strength and stiffness for transportation. This should be considered in developing a bottle design and selecting a polymer.

An aspect that influences the strength of detergent bottles is the potential reaction between the detergent and the polymer. Detergents contain surfactants[1] which can react with the polymer, causing the bottle to crack. In the past reactions have partly been prevented by adding more water to detergents formula or developing polymers with an improved environmental stress crack resistance (ESCR). Currently a trend towards more concentrated products is seen in the market, this will influence the requirements on the polymer in this regard. ESCR will be further addressed in Section 3.3.

Efficient design: Another aspect of transportation is the number of transport movements required for transporting a certain volume of detergent liquid. When a bottle has a 'space efficient' design. Factors influencing space efficiency of the bottle are handles, headspace in the bottle, 'shoulders' on bottles, and curved shapes. Less space efficient bottle designs lead to increased transport movements and therefore result in more CO_2 emissions caused by transportation. This has a negative

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[1] Surface-active-agents. Surfactants are molecules that spontaneously bond with each other to form sealed bubbles. Surfactants lower the surface tension between two liquids, between a liquid and a gas, or between liquids and solids.

effect on the sustainable design goal *Preserve natural capital*. Therefore, when developing a detergent bottle the space efficiency of the design must be carefully considered.

Preserve detergent

Preservation of the detergent is essential. The environmental impact caused by production of the detergent is larger than that caused by the packaging, and thus the primary goal of the packaging is to prevent spoilage of the detergent. A detergent typically has a shelf life of two years. To guarantee this shelf life the detergent packaging must provide the right barrier properties. For preserving detergents the following barrier properties are relevant:

- **Moisture barrier:** Over a long period of time the water in the detergent can condensate and migrate through the bottle, causing the detergent to become less liquid or dry out.
- **Gas barrier:** Some detergents contain hydrogen peroxide which releases oxygen. To prevent build up of pressure in the bottle, resulting e.g. in a deformed bottle, it is desirable that the polymer can passively vent the oxygen.
- **UV-barrier:** Some detergent formulas are sensitive to UV light. UV can cause the colour of the detergent to change, or ingredients in the detergent to separate or break down. This is especially undesirable when detergent is packaged in transparent bottles, as this process will be visible to consumers.

When selecting a polymer for packaging a detergent it is important to consider what barrier properties are required. This can eliminate usage of certain polymers, or require additional additives to provide the barrier properties. In Section 3.2 the barrier properties of different polymers and additives are further explored.

Support dosing

To achieve the sustainable design goal *Prevent product spoilage* correct dosing of the product is essential. Using too much detergent for a cleaning job is a waste of detergent and should thus prevented. The detergent bottle fulfils a critical role in supporting correct dosing of the product.

Handles on bottles: For usability purposes a detergent bottle can contain a handle, enabling easier handling and product by the consumer. As a rule of thumb, according to interviewed brand owners, bottles with a volume larger than 2 litres require a handle for usability and dosing. However, at retailers handles have been found on bottles of 1 and 1,5 litres. As described in the section on transportation, addition of a handle contributes to a inefficient bottle design which requires more transport movements and thus results in in more CO_2 emissions. When designing a detergent bottle it must be carefully considered if a handle is required.

Design considerations

When developing a detergent bottle it must be evaluated what requirements the packaging and selected polymer must fulfil to optimally preserve and transport the detergent:

- Optimise bottle design for efficient transportation to reduce transport movements and thus preserve natural capital. This means excessive curves, headspace and 'shoulders' should be avoided. Additionally it is recommended to only use a handle for bottles larger than 2 litres.

Polymer considerations

Consider what barrier properties are required to preserve the detergent during its shelf life to prevent product spoilage.

Out of scope sustainability aspects in the use phase

Dosing of the product: Using too much detergent is common amongst consumers. Excessive use of detergent has a negative influence on the sustainable design goal *Prevent product spoilage*. Reducing excessive use of detergent is one of the biggest improvements to be made in regard of sustainability. When the volume of detergent used by the consumer is reduced, the use span of a detergent bottle is expanded, resulting in a slower replacement of bottles and thus in a lower volume of plastics.

Concentration of detergent: By increasing the concentration of the detergent, more detergent can be transported in a packaging and thus transport movements are reduced. This contributes to the design goal *Preserve natural capital*. Additionally, less packaging material is required to provide the same number of washes, thus contributing to the design goal *Reduce material use*.

3.2 BARRIER PROPERTIES

The required barrier properties for the detergent bottle depend on the composition of the detergent. Typically, moisture barrier, gas barrier and UV-barrier are relevant to explore when packaging detergents. The considerations for these barrier properties will be elaborated in this section. Table 3-1 provides an overview of the barrier properties of the different polymers.

Moisture barrier

Over a long period of time water in the detergent can condensate and migrate through the bottle, causing the detergent to become less liquid or dry out. Therefore a moisture barrier is required. Commonly used polymers for detergent bottles (PET[2], HDPE and PP) already provide a moisture barrier. This 'natural' moisture barrier is more than sufficient to provide detergents the typical shelf life of 2 years. Thus, in practice it is very rare that producers use additives to enhance barrier properties. Therefore this topic is not further investigated.

Gas barrier

Some detergents contain hydrogen peroxide which releases oxygen. To prevent build up of pressure in the bottle, it is desirable that the polymer can passively vent the oxygen. The polymer matrix of PET is quite solid and provides a good gas barrier, in this case undesirable as the bottle can deform under the pressure that is build up. HDPE and PP are 30 times more permeable to gas than PET and can thus passively vent the oxygen from the bottle[3]. In conclusion, when selecting the polymer for detergents the barrier properties of the different polymers must be carefully considered.

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[2] The moisture barrier of PET is inferior to that of HDPE and PP. When e.g. a laundry detergent is packed in a PET bottle the liquid will dry quicker than when packed in HDPE or PP. A moisture barrier is added in PET bottles for preservation of carbonated drinks. Barriers that are commonly used are for example silicon oxide plasma coating and carbon plasma coatings (European PET Bottle Platform, 2020). As these are not applied in detergent bottles these type of coatings are not further investigated.

[3] https://www.packworld.com/design/materials-containers/article/13347220/pg-pushes-the-limits-of-twostage-isbm

UV barrier

Detergents can be sensitive to UV light. The colour of the detergent can change, or ingredients in the detergent might separate or break down when exposed to UV. This is especially undesirable when the detergent packaged in transparent bottles, as this process will be visible to consumers. Therefore, a UV barrier is required for bottles containing UV sensitive detergents.

Colour additives as UV barrier

PET, HDPE and PP polymers are available as translucent/transparent or with opaque colours. Opaque coloured bottles filter the light and thus provide a UV barrier. In most cases this barrier is sufficient to preserve the detergent. The opaque quality of polymers is obtained by adding pigments (colour additives). When the opaque quality of a bottle is not sufficient a coloured coating can be added. This is not common in packaging. For transparent bottles a full body sleeve can provide a UV barrier.

Adding pigments to HDPE and PP is common practice and - when adhering to some guidelines - has minimal negative consequences in the life cycle of a bottle. However, this is not the case for opaque PET. Opaque PET cannot be fully separated from transparent PET in recycling. Opaque PET in the transparent PET stream will lead to a loss of brightness and transparency, thus reducing the quality, value, and employability of the stream. Additionally, opaque PET cannot be used at the same value but is cascaded to product such as strapping for pallets. Therefore using opaque PET for detergent bottles is discouraged.

Sustainability aspects of pigments are further addressed in Section 5.3 (production) and Section 6.4 (end of use).

UV-barrier in transparent PET bottles

Transparent PET has a very limited light barrier. If UV rays influence the detergent, a barrier can be added. This can be done by adding plastic light stabiliser additives to the resin embedding the barrier in the polymer matrix, or by applying a coating to the blown bottle.

[This part will be further investigated and described]

Table 3-1: Overview barrier properties of different polymers

Polymer	Appearance	Moisture barrier	Gas barrier	UV-barrier
HDPE	Opaque			
	Translucent			
PP	Transparent			
	Opaque			
PET	Transparent	*		
	Opaque	*		

** The moisture barrier of PET is inferior to HDPE and PP, but still adequate for packaging detergents.*

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Polymer considerations

Consider which polymer offers the right barrier properties for packaging the detergent. By selecting a polymer that 'naturally' has the desired characteristics, use of coatings and additives can be prevented. This reduces contamination of the polymer and thus promotes closing the material loop. For example, prefer HDPE or PP polymers for UV sensitive detergents.

Chemical considerations

When improving the barrier properties of polymers for detergent bottles using additives or coatings, consider the following aspects:

- When using additives or coatings, carefully consider how these behave in the bottle. If not embedded in the polymer matrix it can potentially migrate into the detergent.
- A UV barrier can improve the shelf life of a detergent. A UV barrier can be provided by adding pigments to detergent bottles. This prevents usage of light stabiliser additives or UV barrier coatings.
- It is recommended to avoid using colour additives in PET as this compromises the recyclability of the material.

3.3 CHEMICAL RESISTANCE OF POLYMERS

The selected polymer for the detergent packaging must be compatible with the (chemical) ingredients of the formula. In laundry detergents only surfactants will be present. To broaden the relevance and scope of this case study other chemicals present in detergents are also explored. Detergents can contain:

- **Surfactants:** Soaps contain surfactants which react with polymers. This can lead to bottle crack. A good environmental stress crack resistance (ESCR) is thus required in selected polymers, this can be achieved through optimising the polymerisation process. See the paragraph on ESCR for more details.
- **Solvents:** Used in more aggressive detergents. Highly reactive with most polymers, dependent on the aggressiveness of the solvent. PET is unsuitable for packaging solvents. HDPE can withstand mild solvents, but requires fluorine treatment for containing more aggressive variants (e.g. hydrocarbons and aromatic solvents)
  (e.g. aceton) () > fluorine treated HDPE
- **Caustics:** [...]
- **Acids:** [...]

Table 3-2 offers an overview of the chemical resistance of HDPE, PP and PET. HDPE has a good chemical resistance against most chemicals and is the preferred polymer for packaging more aggressive detergents. Chemical resistance of polymers can be enhanced through optimisation of the production process of the polymer (polymerisation) or additives, or the chemical resistance of the packaging can be enhanced through structural enhancement of the bottle (e.g. adding ribs), chemical treatment (e.g. fluorine treatment of HDPE bottles) or a coating.

Table 3-2: Chemical resistance of different polymers

	Surfactants	Solvents	Caustics	Acids
HDPE[4]		Chemical resistance can be improved through fluorine treatment		
PP				
PET[5]				

Fluorine treatment

Untreated, HDPE and PP are sensitive to solvents. However, through fluorine treatment resistance against solving is enhanced.

- "Using a technical process, fluorine atoms are bound to the plastic surface, offering greater barrier properties. This can be done by two processes: in-mold fluorination where the fluorine is mixed with the plastic before being molded, which is not yet FDA approved. The other one called post-mold fluorination and occurs by exposing the bottle or container to fluorine gas in a sealed reactor. Usually it is only the outer surface that is exposed to fluorination, but sometimes fluorination is applied to both outer and inner surfaces, enhancing the barrier properties." [6]
- "Fluorination is FDA safe because it causes a permanent modification to the plastic. It does not wear off or seep into food. Fluorinated bottles are also just as recyclable as any other bottle of the same material."[7]
    - However, fluorine can cause harm to the respiratory system, and irritation to eyes and skin. Additionally it is highly toxic to animals.[8] It should thus be carefully considered if fluorination is required or if other solutions are possible (e.g. in detergent formula or alternative packaging such as glass or metal)
- PET cannot be fluorinated.

Environmental stress crack resistance (ESCR):

Good crack resistance is an essential characteristic of detergent bottles, to facilitate transport of the bottle, storage and usability for consumers. Stress can be caused by various external factors[9]: e.g. top-load stress during transport, internal pressure or through a reaction with other substances. Detergents contain 'surfactants' that react with polymers and can cause a bottle to crack. ESCR is lower for polymers with a high crystallinity – thus lower in HDPE and PP than in PET. For detergents, the following factors around ESCR are relevant:

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[4] https://www.ineos.com/globalassets/ineos-group/businesses/ineos-olefins-and-polymers-usa/products/technical-information--patents/ineos-hdpe-chemical-resistance-guide.pdf
[5] https://roboworld.com/wp-content/uploads/2017/08/PET_ChemicalCompatibility.pdf
[6] https://www.mjspackaging.com/blog/what-are-fluorinated-bottles/
[7] https://www.qorpak.com/pages/Fluorination
[8] https://pharosproject.net/chemicals/2008339#hazards-panel
[9] In the summer, ESCR problems are exacerbated due to several factors related to increased heat and humidity.

- **Polymer development:** Through alterations in the polymerisation process the mechanical specifications of the polymer can be improved. ESCR resistance of HDPE and PE has drastically improved over the past decades through development of polymers and optimisation of the polymerisation process. Development of these polymers includes altering the catalysts and adding a third monomer (propane). These slightly lower the crystallinity of the polymers and thus offer better ESCR.
- **Concentration of detergent:** Highly concentrated detergents contain more surfactants and thus require a higher ESCR of the polymer.
- **Bottle geometry:** ESCR resistance can be improved by optimising the bottle geometry, for example by using a more organic shape and preventing hard edges. However, organic shapes can limit the shape efficiency of the bottle.

Polymer developments have lead to a wide variety of polymer grades with varying mechanical properties. Each polymer that is brought to the market is extensively tested and approved by institutions such as European Chemicals Agency (ECHA). Therefore considerations for sustainability for environment and safety are not regarded as relevant for this case study.

Migration

Migration of the polymer or additives in the polymer to the detergent must be prevented to preserve natural capital and guard the safety of consumers. When substances or chemicals migrate from the polymer into the detergent this can potentially end up in the washing water and thus leak into the sewage system, creating a potential hazard for natural capital. Additionally, detergents come into contact with the consumer's skin when they are being used. However, detergents are always diluted with water. The ppm present in the water would be extremely small and thus do not pose a threat to consumers and natural capital.

In practice, polymers are porous and migration takes place the other way around: detergent substances migrate into the absorbing polymer matrix. Migration is thus not a potential hazard. However, when using additives or coatings on the bottle it is important to carefully consider if leakage can take place and end up in the detergent. If additives are not embedded in the polymer matrix migration can take place. If this scenario is likely, safety of the additives or coating is essential.

Migration of polymer into the detergent

[This part will be further investigated and described]

- "In 2018, research conducted by Sherri Mason from the State University of New York in Fredonia revealed the presence of polypropylene, polystyrene, nylon and polyethylene terephthalate microparticles in plastic bottles. Polypropylene was hereby found to be the most common polymeric material (54%) and nylon the second most abundant (16%) polymeric material. The study also mentioned that polypropylene and polyethylene are polymers that are often used to make plastic bottle caps."[10] These rates were higher than in tap water. Expected to be released from the bottle. What are the consequences?

[10] https://orbmedia.org/sites/default/files/FinalBottledWaterReport.pdf

Polymer consideration

Consider which polymer offers the chemical resistance for packaging the detergent. By selecting a polymer that 'naturally' has the desired characteristics, use of coatings and additives can be prevented. This reduces contamination of the polymer and thus promotes closing the material loop.

Chemical consideration

When using additives or coatings on the bottle it is important to carefully consider if leakage can take place and end up in the detergent. If additives are not embedded in the polymer matrix migration can take place. If this scenario is likely, safety of the used additives or coating is essential. Consult REACH and RSL.

4. SOURCING OF MATERIALS

Relevant sustainable design goals:

1. Reduce material use
    a. Impact of light weighting on sustainability of polymers
2. Close material loops:
    a. Renewability of material or additive source
    b. Recyclability of plastics
3. Preserve natural resources
    a. Biobased plastics
4. Guard health of participants in lifecycle
    a. Safety of used materials and additives

4.1 FEEDSTOCK CONSIDERATIONS FOR DETERGENT BOTTLES

In this first paragraph the overall considerations when selecting a feedstock for detergent bottles are discussed. Depending on the polymer(s) chosen for the detergent bottle, there are three main sourcing routes: primary renewable resources, primary non-renewable feedstock ('virgin'), or secondary feedstock (recycled material).

Renewable resources

A resource is considered renewable when the regeneration is able to keep up with the extraction and consumption of the material. Well known examples are fast growing crops such as corn, sugarcane, sugar beet, and wheat. Rapidly renewable resources are selected to decouple feedstock extraction from fossil resources and to preserve natural capital. Using fast growing crops will also reduce the emission of greenhouse gasses (in comparison with fossil-based resources) as the growth of the plants requires them to capture CO_2 from the atmosphere. The carbon will be stored in the biomass, be converted to a plastic, and eventually will de released back into the atmosphere again as CO_2 or CH_4 (methane) when the plastic is incinerated or decomposes at end of use. A social benefit to the use of renewable resources is that, unlike reserves of fossil resources, their cultivation does not have to be concentrated a certain specific regions in the world. This means that bioplastic production can support local rural economies.

When selecting a renewable resource as feedstock for the plastic, a few sustainability criteria should be considered: land-use change, food scarcity, and agricultural practices. When crops are grown to serve as feedstock for plastic production, arable land is needed. The feedstock is not considered sustainable when it requires the destruction of natural capital, e.g. deforestation of rainforests to gain land. The cultivation of crops for plastic production should also not compete with food production in areas where arable land or water is scarce or crop yields are unstable. By-products or residues of food production can be selected as feedstock in these cases. Furthermore, if the cultivation of the feedstock heavily depends on fossil-based energy, through petrol for tractors and combines for instance, or on the use of fertilizers and pesticides, the overall environmental impact of the feedstock might be higher than that of fossil-based alternatives.

Not all these factors can readily be taken into account in the selection of a polymer to produce a detergent bottle. When a polymer derived from a renewable resource (a "bioplastic") is considered, potential suppliers and the origin of the feedstock should be checked on these criteria.

[Environmental aspects relating to herbicides and pesticides will be further investigated and described]

Primary non-renewable feedstock

Intuitively the fossil-based primary feedstock is regarded as least sustainable. The extraction of the feedstock is polluting and requires the destruction of natural capital. The use of the primary (or 'virgin') material means that the material cycles will not be fully closed and continual extraction of the feedstock is needed. However, the use of primary non-renewable feedstock might be required due to unavailability or incompatibility of materials derived from renewable resources or secondary feedstock. In this case a plastic must be selected that can readily be recycled and the detergent bottle must be designed in a way that enables the highest possible recovery of the material in the existing recycling value chain. In this way the plastic used in the bottle can be reused in another product and replace the need for virgin plastics there. The effects of coating, pigments, and other additives on the recycling potential of the polymer will be discussed in the chapter *End-of-Use*.

A polymer from a primary non-renewable feedstock that cannot be readily recycled, is an unsustainable material and should not be selected for use in a short-lived packaging such as a detergent bottle.

Secondary feedstock

Secondary feedstock, or recycled plastics, can be derived from both renewable and non-renewable resources. The benefit of the use of secondary feedstock is that recovery of the materials after their primary use generally has less environmental and health impact than the production of virgin plastics. Additionally, the use of recycled plastic means that this material is not discarded as waste and the impact of incineration or landfilling has been prevented. The use of recycled plastic in a new product increases the demand for recycled plastics, which makes it more likely that the plastic will be collected and recycled at end-of-use.

- Use of recycled plastics in food applications is very limited, only possible when it can be proven that the source is food grade. To promote the use of recycled materials it is therefore good to use it in non-food applications wherever possible, such as in detergent bottles.
- Using recycled plastics contributes to a circular economy. Same value recycling versus downcycling or cascading.

4.2 FEEDSTOCK OPTIONS

Typically, detergent bottles are made of HDPE, PP or PET. Over the past years it is observed that PP is less frequently selected and a trend towards PET bottles for detergents can be seen. The trend to PET can be explained by the trend of transparent bottles, but also due to the low prices of (virgin) PET. In this case study HDPE, PP and PET will be considered, including their recycled and biobased variants.

The previous section laid out the different sustainability considerations for the different available feedstocks. This section will evaluate how qualified the different feedstocks are for producing detergent bottles. Table 4-3 provides an overview of the different polymer types

Secondary non-renewable feedstock

- Production of detergent bottles is possible with recycled plastics. Examples using 100% recycled HDPE and recycled PET are in the market (see Figure x.x).
    - When necessary, recycled feedstock can be complimented with virgin or biobased feedstock. Aim for highest percentage of recycled possible.
- Production of detergent bottle with recycled PP is not possible. Post-consumer recycled PP comes from injection moulded or thermoformed plastic packaging. These types of packaging is characterised by a high melt flow index (MFI). However, the MFI of recycled PP is too high extrusion blow moulding (EBM) of PP detergent bottles. EBM is the standard production method for PP detergent bottles. Because rPP cannot be used in detergent bottles this material-feedstock combination will not be further explored.
- Common feedstock and availability, see Table 4-1.
    - Transparent rPET is sourced from recycled deposit bottles. This is a food grade source. Using non-food grade transparent flakes is technically possible for production of the bottles, but the supply of these are scarce. What are the consequences of using food grade material? Using food grade material for non-food applications is debatable, because rPET used for non-food applications, cannot be used for food applications anymore. So you are removing resources from a closed loop stream, using them into a stream of which it is often unknown where it ends.
    - Recycled HDPE and PP can be sourced from post-consumer plastic packaging waste.
- CO_2 emissions of recycled plastics is lower than that of virgin plastics because emissions from production of virgin polymers are avoided. Also, recycled plastics promote circularity of detergent bottles. Therefore this is the preferred feedstock for detergent bottles.

Figure 4-1: Detergent bottles made from 100% recycled plastics.
Left: rPET bottle; Right: rHDPE bottle.

Table 4-1: Overview of recycled plastics.

Recycled plastic	Common feedstock	Availability	Suitability for bottle production
rPET	Food grade recycled deposit bottles	Commercial scale	
rHDPE	PCR packaging waste	Commercial scale	
rPP	PCR packaging waste	Commercial scale	MFI is too low for EBM

Renewable feedstock

- Renewable feedstock can be used to complement the use of recycled plastics. Sometimes using 100% recycled is not possible from a technical point of view. Additionally, renewable feedstock can be used as a carrier in the masterbatch, or the production of closures and labels
- See Table 4-2 for an overview of biobased polymers. For HDPE and PET biobased feedstock is widely available.

Table 4-2: Overview of biobased polymers. Based on Siracusa and Blanco (2020)

Polymer	Common feedstock	Availability	Remarks
BioPE	Sugar cane	Commercial scale	
BioPP	Waste cooking oils and palm oil	Scarce	Scarce at time of writing, availability is rapidly increasing
BioPET		Commercial scale	Usually a blend with ± 40% biobased content

Primary non-renewable feedstock

Fossil fuels are not considered to be a sustainable feedstock for detergent bottles. This feedstock is non-renewable and does not contribute to closing the material loop on detergent bottles. Since application of recycled plastic is technically feasible, using primary feedstock in detergent bottles is discouraged.

However, small volumes of virgin polymers can be required. For example as a carrier in the masterbatch and for the production of closures and labels. Additionally, primary feedstock can be used if the technical specifications required for packaging more aggressive detergents cannot be fulfilled using recycled or biobased polymers. Biobased polymers should be preferred as much as possible for these purposes.

Table 4-3: Overview of polymers and their renewability

Material	Renewability of feedstock	Renewability of material	Impact production CO_2/kg[11]
HDPE	Primary fossil based	Recyclable*	2,17
rHDPE	Secondary fossil based	Recyclable*	1,36[12]
PET	Primary fossil based	Recyclable*	3,30
rPET	Secondary fossil based	Recyclable*	2,11[13]
PETG	Primary fossil based	Non-recyclable	*Unknown*
PP	Primary fossil based	Recyclable*	2,19
Bio-HDPE	Renewable resource	Recyclable	-0,16[14]
bioPET	Renewable resource	Recyclable*	*Unknown*
bioPP	Renewable resource	Recyclable*	-1,91[15]
rPP	Secondary fossil based	Recyclable*	1,37[16]

** Provided that the bottle design facilitates recycling.*

Polymer consideration

When selecting a polymer for detergent bottles, consider the following:

- Recycled plastics (secondary non-renewabe) is the preferred feedstock for plastic detergent bottles. By using recycled plastics the material loop can be closed and CO_2 emissions lowered.
- Recycled PET is primarily sourced from food grade deposit bottles. Consider if using food grade material is necessary for a detergent bottle, and if an alternative plastic can be selected.
- Recycled PP is not technically feasible for the production of detergent bottles, therefore production of PP detergent bottles is not regarded as sustainable.
- Renewable feedstock and primary feedstock can be used to supplement recycled plastics to realise desired technical specifications, carrier of the masterbatch, or the production of closures and labels. Renewable feedstock is preferred over primary feedstock because it is a more circular and sustainable option.

[11] Retrieved from the EcoInvent database 3.5 (2018), unless indicated otherwise

[12] Calculation of impact based on the impact of virgin material, the impact of the recycling process and substitution of virgin material, considering the allocation factor and the downcycle factor. All factors are retrieved from the EcoInvent database 3.5 (2018).

[13] Calculation of impact based on the impact of virgin material, the impact of the recycling process and substitution of virgin material, considering the allocation factor and the downcycle factor. All factors are retrieved from the EcoInvent database 3.5 (2018).

[14] Calculation based on values from Chen & Patel (2012) + transport from Brasil to Europe. Does not include effects of land use change.

[15] Calculation based on values from Chen & Patel (2012) + transport from Brasil to Europe. Does not include effects of land use change.

[16] Calculation of impact based on the impact of virgin material, the impact of the recycling process and substitution of virgin material, considering the allocation factor and the downcycle factor. All factors are retrieved from the EcoInvent database 3.5 (2018).

4.3 SECONDARY FEEDSTOCK – RECYCLED PLASTICS

- Conclusion previous section: Use as much recycled feedstock as possible. This section will explore additional sustainability aspects for using recycled HDPE or PET for detergent bottles.

Recycled HDPE

Colour restrictions of recycled HDPE

- Not available in transparent
- Generally less bright colour range is possible compared to virgin
- Colour of rHDPE is improving due to colour sorting technique

Smell of recycled HDPE

Recycled HDPE often has a smell of waste. Polyolefins (PP, PE) have a relatively open structure and when polyolefins are used in (liquid) packaging, substances from the contents can migrate into the polymer matrix. The rate of migration strongly depends on the size of molecules, if smaller then more can migrate. The migration process follows Fick law and is therefore also depending on time. In mechanical recycling of HDPE detergent bottles migrated fragrances cannot be removed completely in the washing process. By extrusion with a vacuum exhaust plastic flakes are converted into pellets and part of the volatile fragrances are removed. However, the a slight smell remains. Often this can be the reason a recycled polymer is rejected for the production of new bottles. Because detergent formulas often have a strong smell of themselves it is recommended to test the rHDPE bottles when filled with the detergent. It is very likely that the scent of the detergent cancels out the rHDPE smell. Also, over time the detergent scent will be absorbed in the polymer matrix of rHDPE.

Regulations on using recycled material

[This part will be further investigated and described]

Impurities in the HDPE stream

rHDPE streams can contain small contaminations, originating from product residues in the packaging waste stream, such as organic waste, cosmetics or detergents. But also surfactants, plasticizers and solvent polymers can be found. According to Horodytska (2020) pollutants are well below the norms and will not cause any health risks or impact recycling. Also recycled HDPE nearly always contains some PP, for example from the closures used on detergent bottles. For most applications this is not an issue; up to 2-3% PP can be allowed. In sourcing recycled HDPE for bottles this should be taken into consideration: How clean should the rHDPE stream be? Because PP in recycling streams usually have a higher MFI, presence of PP in rHDPE might influence the processability of the feedstock in EBM. Evaluation of the production process is required to determine the allowed contamination.

Improving quality of recycled HDPE

HDPE polymers degrade in quality by heating in the compounding process. This can be countered by adding processing stabilizers (anti-oxidanten).

[This part will be further investigated and described

Masterbatch composition for recycled HDPE

- Overview of masterbatch composition

Recycled PET

Characteristics of recycled PET

[This part will be further investigated and described]

Impurities in the PET stream

[This part will be further investigated and described]

Improving quality of recycled PET

- **Anti-yellowing agents:** rPET degrades in quality by exposure to heat and impurities in the recycled PET stream[17]. This results a yellowish colour tone of the material. The colour has no further negative effects, but is not desirable in terms of aesthetics. Anti-yellowing masterbatch can be added in the process to neutralize the visual effect[18]. These additives are not pigments and do not affect the recycling.
- **Solid state polymerisation and melt enhancing additives:** Another effect is that in recycled PET the quality expressed as IV (Intrinsic Viscosity) is lower. rPET will break down in smaller polymer chains. The ester group in the molecules is than hydrolysed. This can be restored by Solid State Polymerization (SSP) or usage of additives. SSP is the reaction of PET molecules in PET pellets. Required are a high temperature (> 210 °C) and high vacuum. The reaction is an equilibrium reaction and by removing moist the this equilibrium is supported in the direction of longer molecular chains of the polymer. Melt enhancing additives in the masterbatch support a uniform cell structure and improves mechanical performance and processing stability[19]. How much masterbatch is required depends on its application.

Polymer considerations
[...]

Chemical considerations
[...]

4.4 CHEMICAL ADDITIVES IN PRODUCTION OF PLASTIC RESIN

Use of virgin plastics (primary non-renewable feedstock) cannot be completely avoided. Therefore, this section will consider the sustainability aspects on a chemical level of the production of virgin resin. Virgin plastics are e.g. required as a binder in the masterbatch, but can also be used to upgrade the quality of recycled plastics when this is inadequate.

Production residues

[17] https://www.sukano.com/en/applications/rpet
[18] https://www.ampacet.com/blueedge-formula-x-pet-bottle-brightener/
[19] https://www.sukano.com/en/applications/rpet

Two main processes are used to produce plastics - polymerisation and polycondensation - and they both require specific catalysts. In a polymerisation reactor, monomers such as ethylene and propylene are linked together to form long polymer chains. Each polymer has its own properties, structure and size depending on the various types of basic monomers used.[20]

Monomers are the starting molecules that are used to form a polymer through polymerization, or the product of degradation of a polymer after production. A well known restricted monomer is Bisphenol A (BPA) an endocrine disrupting chemical (EDC) and a migration limit for the substance is set in EU regulation since 2018. Monomers are not expected in polyolefins as these are very volatile substances that are separated from the polymer pellets produced.
[Monomer in PET will be further explored]

Oligomers are partially reacted monomers or degradation of polymers. They are mainly found in polyesters (PET). Oligomers can be present in polyolefins as waxes. *[to be further researched]*

Catalysts are chemicals that start or accelerate a chemical reaction. In this case, the polymerisation from monomers to polymers. In the production PP catalysts can be added that are formed from a 'pre-catalyst mixture' containing, among other substances, phthalates. It forms the catalyst in the reactor in which the polymerisation will take place. Phthalates such as DEHP have endocrine disrupting properties. These phthalates are usually consumed in the reactions, but traces can be left in the final PP. Most impurities are removed in the purification stage and test are performed to determine that concentrations are below specified limits.

Additives in primary feedstock

Additives are used to make plastics easier to process, enhance its mechanical properties (such as impact or stress crack resistance) or give it specific aesthetic qualities. In general few additives are expected to be used in plastics for detergent bottles. Detergent and bottle producers indicated that only colourants are added, and in some cases additives to provide a UV barrier (PET bottles). Additives require an additional financial investment. Therefore producers try to avoid these where possible to cut costs.

Nevertheless, this section will briefly consider additives that could potentially be present in plastic resin for detergent bottles. Table 4-4 provides an overview. A distinction is made between functional additives that alter polymer characteristics, additives used to optimise production processes of e.g. bottles, and additives that are added to alter the appearance of a plastic. Additives for production and aesthetics are discussed in Section 5.3.

[20] https://www.plasticseurope.org/en/about-plastics/what-are-plastics/how-plastics-are-made

Table 4-4 Potentially relevant additives for detergent bottles[21]

Functional additives	Additives used for production*	Additives for aesthetics*
Flame retardants	Antistatic agents	Pigments
Heat and oxidation stabilisers	Slip agents	Fillers**
Biocides	Lubricants	
Plasticisers		
Impact modifiers		

** Further elaborated in Section 5.3.*

*** Fillers are not always used for aesthetics only, but this is the relevant functionality for this case study.*

Flame retardants reduce the flammability of plastics. Many flame retardants have been banned due to reprotoxicity and carcinogenic toxicity and endocrine disruption. They are not added to resin for the application in plastic bottles.

Heat and oxidation stabilizers are used in PP, PE, PS, PA, PET to prevent polymer degradation in extrusion. *[will be elaborated upon: examples of banned or suspected stabilizers]*

Biocides prevent the degradation of plastics from microbiological attacks. It might be used to slow down biodegradation of biodegradable plastics, so not relevant for this application.

Plasticisers *[This part will be further investigated and described]*

Impact modifiers *[This part will be further investigated and described]*

Chemical considerations
Chemicals additives are added to the virgin plastic to serve specific purposes but can have consequences for the sustainability of the plastic product. They might hamper recyclability or pose a toxicity risk to human health or biodiversity at any point in the lifecycle. It should be considered whether the addition of the chemicals to the plastic is indispensable or whether more sustainable alternatives can be chosen.

[21] https://www.bpf.co.uk/plastipedia/additives/default.aspx#AdditivesRespect

5. PRODUCTION

Relevant sustainable design goals:

1. Prevent product spoilage
2. Reduce material use
    a. Influence of material choice on volume of material required
    b. Impact of production method on material use
2. Guard the safety of production workers
    a. Chemicals used in production
    b. Additives required for production

5.1 PRODUCTION METHODS

In this paragraph the commonly used production methods for detergent bottles are described. The production process as indicated in Figure 5-1 is used as an outline.

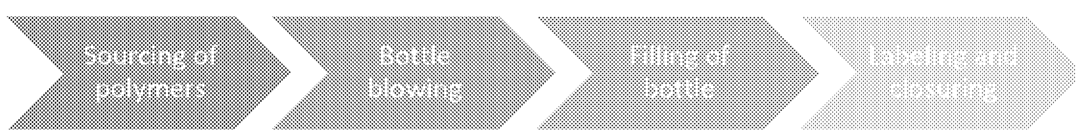

Figure 5-1: Production and filling process of detergent bottles

Common production methods for detergent bottles are extrusion blow moulding (EBM) and injection stretch blow moulding (ISBM), other production methods are not common practice for large detergent producers. The two production methods will be briefly explained below, see Table 5-1 for an overview.

Extrusion blow moulding

In extrusion blow moulding (EBM) a parison is extruded over which a mould is closed (see Figure 5-2 for production overview). Subsequently, the parison is blown into the mould to shape the bottle. Finally, the trims caused by production are removed. EBM allows the creation of a handle on the bottle, which cannot be achieved using ISBM. EBM requires a low melt flow index (MFI), and therefore HDPE and PP are most suitable for this production process.

In EBM different layers can be co-extruded. In this way recycled layers en virgin layers can be combined. This can be desirable for giving the bottle a 'virgin look' while simultaneously increasing the recycled content. Also, this approach can reduce the need for pigments in a bottle by only colouring the outer layer.

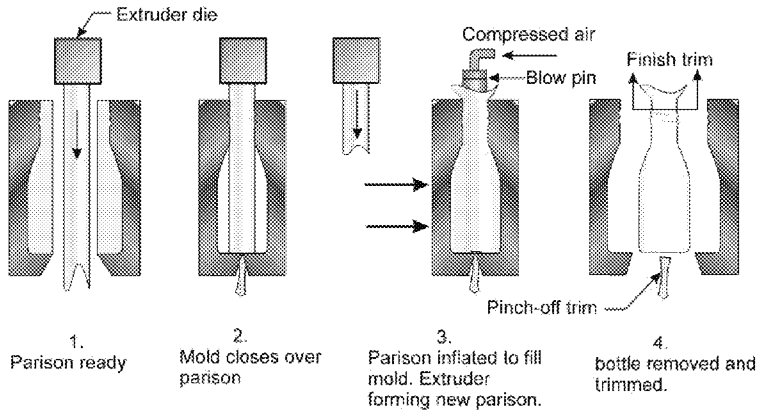

Figure 5-2: Extrusion blow moulding production process

Injection stretch blow moulding

Injection stretch blow moulding (ISBM) consists of two steps: first a preform is produced using injection moulding, after which this preform is blown into a bottle mould creating a bottle. These two steps can be executed in one process, or the preform can be purchased externally and reheated before bottle blowing. The latter can prevent emission to the environment due to transporting empty bottles. ISBM is a more expansive process than EBM, but allows for more form freedom. However, it is not possible to create bottles with handles using the ISBM technique. Generally ISBM is used to produce PET bottles.

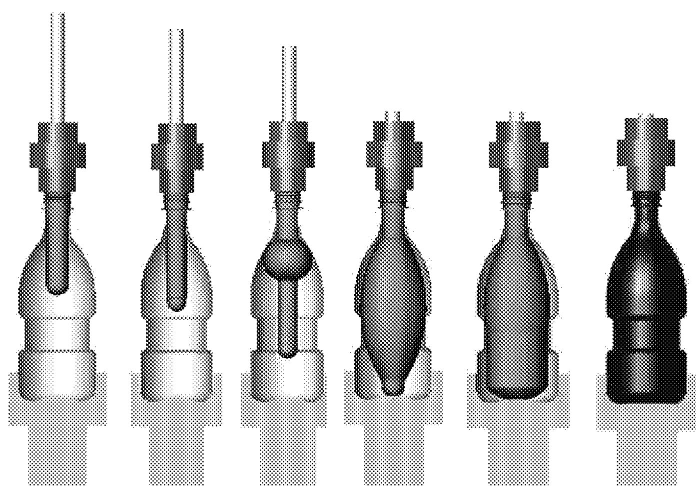

Figure 5-3: Injection stretch blow moulding production process

Table 5-1: Overview production methods

Production method	Characteristics
Extrusion blow moulding	- Enables handle on bottle - Less freedom of form - Cheaper than ISBM - Emissions at production approximately: 1,47 CO_2/kg
Injection stretch blow moulding	- Handle on bottle not possible - More accurate, more precise measure tolerance - Expensive compared to EBM - Emissions at production approximately: 1,95 CO_2/kg

Filling

The blown bottle can be filled with a detergent. This filling process has no further implications for the sustainability of the bottle design and will thus not be further elaborated. An aspect that must be considered is the transportation distance between the production facility where the bottles are blown and the location where the bottles are filled. Ideally, bottles are blown and filled at the same location, with limited distance to retailers. When bottle blowing and filling is not possible at the same location, it is recommended to consider the environmental impact of transportation of empty bottles versus reheating preforms for ISBM blow moulding. This could be a factor that influences polymer selection.

5.2 POLYMER SELECTION

Not all polymers can be used for all bottle blowing production methods. Table 5-2 provides an overview of the suitable production methods for the different polymer feedstocks.

HDPE

HDPE bottles can be produced using extrusion blow moulding. HDPE can be sourced from (a combination of) recycled, renewable or virgin feedstock. EBM of different polymer feedstocks is feasible without the addition of additives or other enabling substances in production. Recycled and biobased polymers will behave differently in production, but there can be compensated for this by adjusting the settings of the machines.

PP

For the production of detergent bottle PP is usually blow moulded. However, extrusion blow moulding of PP is not possible when this is sourced from a recycled feedstock (preferred feedstock for detergent bottles, see Chapter 4). Most PCR PP comes from injection moulded or thermoformed plastic packaging. Typically, these have a high MFI, opposed to the low MFI required for EBM. Therefore recycled PP is characterised by a high MFI. rPP with a low MFI is difficult to source, and therefore is not adopted by producers to make bottles using EBM. Consequently, the material loop of PP is difficult to close for the application in detergent bottles. Therefore PP will not be further investigated in this case study.

PET

PET detergent bottles are produced using ISBM. The melt flow index of PET is too high for EBM. PET can be sourced from (a combination of) recycled, renewable or virgin feedstock. ISBM is feasible without addition of additives or other enabling substances in production. Recycled and biobased polymers will behave differently in production, but there can be compensated for this by adjusting the settings of the machines.

In general less material is required for ISBM of a PET bottle compared to EBM of an HDPE bottle of the same volumes.

Table 5-2: Overview of polymer and possible production methods for detergent bottles

Polymer	Extrusion blow moulding	Injection stretch blow moulding
HDPE		Not generally applied
rHDPE		MFI too low
bioHDPE		Not generally applied
PP		Not generally applied
rPP	Difficult to obtain grade with low MFI	Not generally applied
bioPP		Not generally applied
PET	MFI too high	
rPET	MFI too high	Bottles made from 100% rPET are on the market
PETG		

Polymer consideration

- By using layers in extrusion blow moulding the bottle recycled content can be increased by only using virgin material in the outer layer. Also the need for pigments can be reduced as these are only required in the outer layer of the bottle.
- PP bottles can not be produced using recycled feedstock. Therefore development of PP bottles is discouraged.
- The production of PET bottles requires less plastic (in kg) compared to HDPE bottles of a similar volume.

5.3 ADDITIVES AND CHEMICALS USED IN PRODUCTION

This paragraph describes the additives used as ingredients in the production of the bottles, such as pigments used in the masterbatch, and additives or other substances that support the production process, such as lubricants and anti-statics.

Pigments

Pigments are only considered for extrusion blow moulding of HDPE. Coloured PET is not accepted in recycling[22] , therefore pigments used for this purpose are not relevant. Pigments are added to the 'masterbatch'. This masterbatch is mixed with the polymers in the extruder. In general a masterbatch consists for 5-10% out of pigments, the remainder is virgin polymers. In a virgin bottle 2% is required on average. In general recycled bottles require a higher percentage of masterbatch (e.g. 3% is used in detergent bottle made with 97% PCR rHDPE)

[22] rPET can be recognized by its grey haze. This is caused by pieces of coloured PET that pollute the material stream. As rPET is predominantly used in transparent, uncoloured applications, such pollutants must be avoided. This can be achieved through only producing transparent, uncoloured PET. In this way a closed material stream can be realised.

Depending on the desired colour a pigment is selected. In general, the bottle producer mixes the pigments with the natural resin (either virgin, biobased or recycled) just before blowing the bottle. Commonly used pigments are for example titanium dioxide (TiO_2) to create a white colour and carbon black to create a black colour.

Safety of pigments

Pigments are colored, insoluble chemical compounds with the ability to give color to another material. In plastics, pigments are dispersed within a binder matrix (masterbatch), which is then added during compounding of the granules to imbue it with colour. "Pigments keep their original shape (as small crystals) over the complete life cycle, a consideration that must be taken into account during the material health assessment process" (Cradle to Cradle Products Innovation Institute, 2019).

Pigments can be divided into two groups (Cradle to Cradle Products Innovation Institute, 2019):

1. **Inorganic pigments:** Inorganic pigments, often metal oxides or metal sulfides, usually show high light fastness and temperature stability, but often limited brilliance. Important inorganic pigments are titanium dioxide, iron oxide, zinc oxide, zinc sulfide, barium sulfate, chromium(III) oxide, cobalt blue, lead oxide, cinnabar and cadmium yellow.
2. **Organic pigments:** Similar to dyestuff molecules, organic pigments can be classified according to their chemical structure. Classes of organic pigments include: Azo pigments, Disazo pigments, Polycyclic pigments, Anthraquinone pigment, Dioxazine pigments, Triarylcarbonium pigments, Quinophthalone pigments. Azo pigments are the commercially most important group of organic pigments

Organic pigments have a superior environmental profile in comparison to inorganic pigments and provide a wider range of bright colors.[23]

"Several toxicity studies have been performed on pigments for select hazard endpoints including acute toxicity, mutagenicity, and irritation potential[24]. The results showed that very few pigments are hazardous. The main reason for this is that most pigments are poorly water soluble and predominantly chemically inert, and as a consequence are not bioavailable. In colored plastics pigments are embedded in a matrix and therefore exposure is limited." (Cradle to Cradle Products Innovation Institute, 2019)

However, safety of added pigments should be carefully considered. This can be done by consulting if a pigment is REACH compliant or present on the *Restricted Substances List* from the *Cradle to Cradle Institute*. However, additional steps can be taken to ensure safety and sustainability of pigments, by following *Colorants (Textile Dyestuffs and Pigments) Assessment Methodology* required for Cradle to Cradle certification. It will then be assessed if a pigment is chemically stable or whether they have the potential to form hazardous reaction products. For pigments used at a concentration of >100ppm in detergent bottle the following rules apply (Cradle to Cradle Products Innovation Institute, 2019):

- **Organohalogens:** pigment containing a covalent fluoro-carbon, chloro-carbon, bromo-carbon or iodo-carbon bond should be avoided.

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[23] https://www.pcimag.com/articles/87442-u-s-color-pigment-demand-to-reach-3-8-billion-in-2011
[24] Wiley: ULLMANN'S Encyclopedia of Industrial Chemistry. John Wiley and Sons, Inc. NY 2014

- **Toxic elements:** Pigments containing lead, cadmium, mercury, vanadium, chromium(VI), cobalt, nickel, arsenic, antimony or selenium should be avoided.
- **Reductively cleavable aromatic amines:** An azo pigment containing one or more carcinogenic aromatic amines as defined in European regulation 76/769/EEC should be avoided.

Note that REACH compliance or Cradle to Cradle certification does not automatically clear the pigment for usage in detergent bottles. The Carbon black pigment, for example, is C2C bronze certified[25]. However, as will be laid out in Section 6.2, use of carbon blacks inhibits correct sorting of the packaging and thus prevents its recycling.

Additional chemicals used in production - Lubricants and antistatics

In the production of bottles, lubricants and antistatics can be used to release bottles from their moulds. Lubricants are used to ease processing and reduce cycle times. They may also have a positive effect on surface quality of a product. In HDPE metal salts of stearates can be used as an internal lubricant, these types of products are in the positive list of EU no 10/2011. Lubricants are only required for complex geometries, bottle producers indicate it is rarely used for releasing detergent bottles from their moulds. Additionally, antistatic additives are probably not used in packaging products as there is no real need for that.

Chemical considerations

- Prefer organic pigments over inorganic pigments.
- Most pigments do not have health consequences because they are embedded in the polymer matrix and therefore exposure is limited.
- Avoid using halogen-containing pigments because the combustion products at incineration are toxic. Pigments containing a covalent fluoro-carbon, chloro-carbon, bromo-carbon or iodo-carbon bond should be avoided.
- Pigments containing toxic elements such as lead, cadmium, mercury, vanadium, chromium(VI), cobalt, nickel, arsenic, antimony or selenium should be avoided.
- Azo pigment containing one or more carcinogenic aromatic amines as defined in European regulation 76/769/EEC should be avoided.

[25] https://blackbearcarbon.com/2017/06/29/black-bear-debuts-worlds-first-cradle-cradle-certified-carbon-black/

6. END OF USE

This phase includes disposal of the packaging by the user, sorting of the packaging and recycling of the materials. This phase touches upon three of the overarching sustainability goals:

1. **Close material loops:** In a relatively low-tech packaging as detergent bottles closing the material loops is feasible. This means the recycled product of a detergent bottle should be reusable in the production of new bottles (bottle-to-bottle recycling).
2. **Preserve natural capital:** In end of life littering of the packaging should be prevented at all times. Additionally, pollution caused by mechanical recycling, chemical recycling or thermal recycling must be prevented.
3. **Guard health of participants in lifecycle:** The end of life stage should be safe to all involved. This includes safe disposal by the user and safe recycling processes for workers, without exposure to unsafe or toxic substances.

End of use scenarios

In the chemical selection for a plastic packaging it should be taken into account how the packaging will most likely be processed at End of Use (EoU). The available waste infrastructure will *steer* the choices that need to be made: the design of the packaging must fit the most sustainable option for processing at End of Use. This includes collection and sorting of the packaging required before any of the aforementioned processes. In case of recycling, the material must be able to be recovered in the best possible quality to be reused in a new product or packaging. In all scenario's, exposure of waste management workers to hazardous chemicals or emissions of hazardous substances to the environment must be prevented. Emissions of greenhouse gasses should be limited.

End of Use scenario to be considered

There are two End of Use (EoU) scenarios to be considered for detergent bottles: Mechanical recycling or incineration and landfilling. Both scenario's start with disposal of the detergent bottle, this is elaborated in section 6.1 on waste collection.

Out of scope

The following EoU scenarios are regarded as out of scope:

- **Chemical recycling:** "Chemical recycling is a process which converts polymeric waste by changing its chemical structure to produce substances that are used as raw materials for the manufacturing of new products, which excludes production of fuels or means of energy generation. Chemical recycling is complimentary to mechanical recycling and can offer a solution to difficult to recycle or non-recycled plastics such as multi-layers, heavily contaminated waste, or mechanical recycling residues." (Plastics Recyclers Europe, 2020) Detergent bottles are made of a mono-material and are suitable for high-value mechanical recycling. Chemical recycling of detergent bottles will recover less value of the invested materials and is therefore not further investigated.
- **Composting:** The composting of a plastic packaging requires the packaging to be made of a biodegradable polymer. As discussed in Section 4.2 this feedstock is not considered for detergent bottles.

- **Littering:** Littering of plastic packaging has detrimental effects on the environment but is not considered as an EoU scenario in this case study. Detergent bottles are not commonly littered by consumers as they serve a clear indoor purpose and are subsequently disposed of with the household waste streams.

6.1 WASTE COLLECTION

When discarded properly by the consumer, the detergent bottle can be collected through three main routes. Which route the packaging follows depends both on locally accessible collection system and the consumer behaviour. The disposal routes of residual waste, separated plastic packaging waste , and post-separation are briefly explored below.

[Insert image of disposal routes]

Residual waste

Most plastic packaging is currently disposed of with the municipal waste collection of residual household waste. This means that the detergent bottles are mixed with food scraps and other unsorted materials. It might be sorted-out for recycling in a so-called post-separation plant, also sometimes called a post-collection separation plant. However, in most countries this is not common practice. Unsorted residual waste is either incinerated or landfilled.

Separated plastic packaging waste

If available, the detergent bottle can be discarded by the consumer through the separate collection of plastic packaging waste, pre-sorted from the residual waste by the consumer at home. Rigid plastic bottles are easily recyclable and in most countries a collection system is in place. How this system is organised varies a lot between countries; from collection at the homes of consumers to central collection points where a consumer can bring the pre-sorted packaging. After collection the waste stream, including the detergent bottles, needs to be sorted in one of the material streams for further recycling, this is further elaborated in Section 6.2.

Post-separation

Recent technological developments allow for separation plastic packaging waste from mixed residual waste in post-(collection-)separation facilities. Availability of these sorting facilities is not widespread at the time of writing (late 2020). After sorting, the separated plastic will be transferred to plastic recycling plants or might be sorted a second time in plastic sorting facilities into different polymer streams.

Plastic recycling rates

The rates of plastic recycling very significantly per country, waste stream, and polymer type. It is striking that recycling rates for PET and HDPE often exceed 10%, whereas recycling rates for PP are close to zero (OECD, 2018). PET and HDPE are used in large quantities for (food) packaging which is better recycled in general compared to other applications. Volumes of rigid PP packaging are quite low and therefore not generally recycled. This motivates the use of PET or HDPE polymers in detergent bottles, as recycling at end of use is better developed for these polymer types.

Recycling rates for clean, high value plastics found in rigid packaging are generally higher than e.g. film packaging. The plastics can be easier repurposed and are interesting from an economical perspective. Therefore, it is expected that recycling rates for plastic detergent bottles are higher than average.

Polymer consideration

In the selection of a polymer the End of Use scenarios should be considered. Determine what disposal routes are available for the packaging and to which EoU scenarios this will lead: mechanical recycling or incineration and landfilling.

- When mechanical recycling is available, make sure a polymer is selected that is mechanically recycled in the region, and optimise the packaging for recycling.
- When mechanical recycling is unavailable, the material loop cannot be closed. Focus on reducing the environmental footprint of the packaging as much as possible, to preserve natural capital.

6.2 SORTING - RECYCLABILITY OF PACKAGING DESIGN

Plastics that are either pre-separated in households or separated from the residual waste after collection, need to be sorted in a few main polymer 'streams' before they are fit for recycling. The sorted and recycled streams vary per country. Usually rigid PET, HPDE and sometimes PP are sorted as individual streams.

To create clean mono-streams sorting of the packaging and polymers (a combination of) several techniques can be adopted. Which technique is applied depends on how technologically advanced the recycling facility is. Often, plastic streams are sorted multiple times to create a high quality mono-stream. The sorting process is roughly as follows:

1. **Sorting packaging in mono-streams:**
   a. **Near-infra-red (NIR):** NIR scanners positioned above the conveyer belts detect the polymer type of a packaging using infra-red technique. Based on the identification the packaging is sorted in a mono-stream, for rigid plastics usually rigid PET and HDPE, sometimes PP.
   b. **Digital watermarking:** A recent development in the sorting of plastic packaging waste. Watermarks are added to the label of a packaging or by applying a 'digital watermark', which can be printed on the label (shrink sleeve, in-mould label, paper or other material) or physically incorporated as a subtle pattern embossed in the plastic itself. The watermark is read and provides the sorting system with information unique to that item by pointing to a database where that information is stored. The information tells the system in which way to sort the item[26].
2. **Shredding packaging into flakes**
3. **Washing of flakes:** The flakes are washed to remove contamination of the stream, for example from organic waste and product residues, and remove labels, adhesives and ink.

[26] https://www.newplasticseconomy.org/assets/doc/Holy-Grail.pdf

The washing step is essential in creating a clean polymer stream. Water temperature and detergents used depend on recycling facility and material stream. Usually ended with rinsing the flakes of all detergents.

4. **Flake sorting:** So far the packaging has been sorted into mono-streams. However, the stream is still contaminated by other polymers, for example caused by closures that were attached to the detergent bottle at disposal. Flake sorting varies per polymer stream:
    c. **Sink float for PET:** The density of PET is higher than that of PP and PE; in water PET will sink whereas PP and PE will float. This principle is used to sort out PET flakes.
    d. NIR flake sorting for HDPE

[insert image of sorting process]

Bottle design influences correct sorting of the packaging

To enable correct sorting of a detergent bottle the complete packaging design, including closures, labels and adhesives, must facilitate the common sorting process that is in place. This section evaluates the complete design of the detergent packaging and highlight which design considerations influence sorting of the plastic bottle per sorting step. There is differentiated between HDPE and PET bottles as these have different requirements.

Sorting packaging in mono-streams – Correct use of labels

Incorrect usage of labels inhibits correct sorting of the bottle using NIR technology[27]. When the surface area of the label is too large the NIR will sort the bottle based on the material of the label rather than the material of the bottle. When these are not made of the same material the bottle will end up in the wrong recycling stream. This problem is well known amongst full body sleeves[28]. In the table below guidelines for correct usage of labels can be found for HDPE and PET bottles. Additionally, it must be noted that PVC labels must be avoided. PVC labels compromise sorting using NIR and result in impurities in the recycling stream.

Table 6-1: Label guidelines for HDPE and PET bottles, based on KIDV (2019), RecyClass (2020)

Bottle material	Label material	Label size*	Sortable with NIR	Recyclability of bottle-label combination
HDPE	PE	Not relevant because same polymer as bottle	Yes	Yes
	Paper	Not relevant because paper interferes with PE recycling	No	No
	PP or PET	<50% for <500ml <70% for ≥500ml	Yes	Yes
		>50% for <500ml,	No	No

[27] NIR is a standard in most recycling plants and thus used as a benchmark.

[28] A full body sleeve can enable the usage of a clear bottle as it also functions as a UV-barrier.

		>70% for ≥500ml		
PET	PET	Not relevant because same polymer as bottle	Yes	No**
	Paper, PE, PP	<50% for <500ml <70% for ≥500ml	Yes	Yes
		>50% for <500ml, >70% for ≥500ml	No	No

** See* Figure 6-1 *for and illustration of the label sizes.*

*** PET labels (films) pollute the recycling of rigid PET. This is predominantly because the labels are heavily printed and the inks influence the colour and transparency of the rPET.*

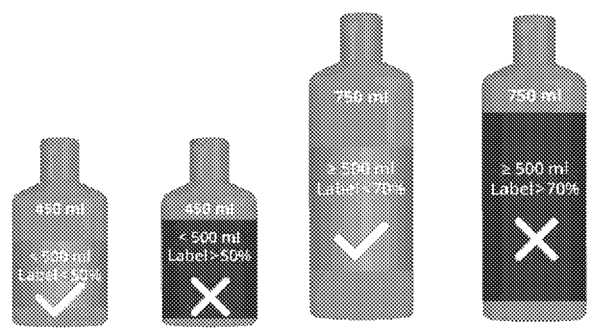

Figure 6-1: Guidelines for label sizes (KIDV, 2019)

Sorting packaging in mono-streams – Pigments

To create dark coloured bottles often the pigment carbon black is used. However, presence of carbon black in a plastic packaging inhibits detection of its material by NIR scanners. Carbon black strongly absorbs infrared radiation as well as visible light, so the NIR light is not reflected into the detectors. Packaging containing carbon black pigments are therefore not sorted into mono-streams and end up in the mix-stream or are incinerated.

Sorting packaging in mono-streams – Watermarking

The introduction of Section 6.2 briefly introduced the concept of watermarking, which is part of the HolyGrail project. The watermark provides the sorting system with information unique to that item by pointing to a database where that information is stored. The information tells the system in which way to sort the item[29]. A lot more information can be collected from a watermark than data that is collected using NIR technology. One of the important benefits is that it enables separation of food grade from non-food grade packaging. This can create a food grade recycled HDPE feedstock. Also, rPET used in non-food applications can be separated from food grade applications.

At the moment of writing the HolyGrail project is making rapid progress. The first sorting plants are installing the required scanners above the sorting lines. It is therefore recommended that in the design of new detergent bottles this digital watermark is incorporated. The watermark can be printed

[29] https://www.newplasticseconomy.org/assets/doc/Holy-Grail.pdf

on the label (shrink sleeve, in-mould label, paper or other material) or physically incorporated as a subtle pattern embossed in the plastic itself. The latter can be realized by embossing the mould used for blowing bottles.

Shredding process – Metals in packaging

When the bottles are sorted into HDPE and PET mono-streams the packaging is shredded into flakes. As a general guideline metals must be avoided in packaging, as this can damage the recycling installation (RecyClass, 2019). Metals are often applied in closures, such as springs in spray nozzles. As closures are often attached to the bottle at disposal these will end up in the mono-streams. Subsequently their design must be considered.

Washing process – Correct use of adhesives for fastening labels

Once the detergent bottle is sorted in the HDPE or PET mono-stream, the bottle is shredded into flakes and washed to remove residues of the product, organic waste, labels and adhesives. Adhesives are used to secure labels to the detergent bottles. The adhesive must dissolve to release the label from the bottle. When the adhesive is not selected correctly it can pollute the recycling process, for example by giving the recycled material a yellow hue or by creating gels in the process. Especially hotmelts and pressure sensitive adhesives cause problems in recycling. The adhesive should be selected so that it is washed off during the washing step in the sorting process. This depends on the water temperature and detergents used in the washing process. In the table below guidelines for selecting adhesives are shown.

Table 6-2: Adhesive guidelines for HDPE and PET bottles (RecyClass, 2020) (RecyClass, 2020)

Bottle material	Adhesive soluble or releasable in	Washing temperature
HDPE	Water	<40°C
PET	Alkali / Water	60-80°C

Flake sorting – Design of closures

In the aforementioned steps the packaging is sorted into mono-streams, shredded and washed. A mono-stream can be contaminated by other polymers. For example caused by the closures used on bottles[30]. When these are attached to the bottle at disposal these will end up in the mono-stream of the bottle polymer. Closures on HDPE and PET bottles are often made from PP, which thus contaminates the HDPE or PET stream. To increase the purity of a mono-stream additional sorting steps can be applied, such as sink-float for PET streams and NIR flake sorting for HDPE streams.

- **Sink-float of PET stream:** This sorting method is based on the principle that the density of PET is higher than that of PP and PE. This means that PET will sink in water whereas PP and PE will float. To ensure a pure PET stream it is important that no fillers are used in PP or PE closures, because this alters the density of the polymer[31]. If the addition of fillers increases

[30] In general closures are made from a different polymer than the bottle because the materials must have a different hardness to provide a solid closure without needing an inlay. For HDPE bottle PP closures are commonly used. For PET bottles both HDPE and PP are suitable. In the past PP was used more, but now a trend towards HDPE closures is seen.
[31] Use of MICA (pearl effect) or metal flakes (metal effect) in caps and closures is common in detergent packaging to give a more high-end look and feel tot he product.

the density of PP or PE above 1g/cm^3 the polymer will sink along with the PET, polluting the stream.

- **NIR flake sorting of HDPE stream:** Closures are generally made from PP. HDPE and PP have a similar density and can thus not be separated from each other using sink-float sorting. This means PP can potentially end up in the HDPE stream. Innovative recyclers have a NIR flake sorter in the sorting process. This means that PP from closures can be separated from the HDPE stream, to minimize PP content in PE.

Design considerations

When a bottle is mechanically recycled, investigate the local sorting and recycling process. In general, when mechanical recycling is considered the following design rules need to be adhered to, to allow sorting of the plastics in a bottle in clean mono-streams:

- **Labels:** Avoid the use of full body sleeves and PVC labels.
- **Labels:** Select the material and size of the label to enable correct sorting of the detergent bottle.
- **Closures:** Avoid fillers in PP and HDPE closures that increase the density above 1g/cm^3 to enable the closure material to be separated from the plastic bottle. Use of fillers in PP and PE can increase the density of the polymer, causing it to sink instead of float. The recycling process is based on the floating property of PP and PE.
- **Adhesives:** Select adhesives for the label that are soluble or releasable in the washing process.
- Apply a watermark to the label or bottle to allow sorting of the packaging as part of the HolyGrail project.

Chemical considerations

When mechanical recycling is considered, the following rules need to be adhered to:

- **HDPE and PP:** Ensure the density of HDPE and PP used in bottles is not above 1g/cm^3. Otherwise the plastic will not be sorted for recycling. Thus, use a mono-material and avoid fillers.
- **Pigments:** Avoid using carbon black as a pigment, because it prevents corrects sorting of detergent bottles and thus inhibits recycling.

6.3 MECHANICAL RECYCLING - RECYCLABILITY OF PLASTICS

The previous section elaborated how detergent bottles are sorted, shredded and washed resulting in mono-stream materials, in this case PET and HDPE streams. This paragraph reflects on the recyclability of the resulting polymer streams. First, a brief overview of the process of mechanical recycling is given:

1. Starts with a (colour sorted) polymer mono-stream
2. Compounding regranulate
    a. Mixing and melting
    b. Adding additives
        i. Stabilizers
        ii. Masterbatch: pigments
    c. Extrusion and granulation > end product ready for production of new bottles

Quality degradation of polymers in recycling

In mechanical recycling polymers are melted and reworked to regranulate. This process results in a degradation of quality of the polymers, as the polymers break down at high temperatures in an extruder. This is on a microscopic scale and often not detected on a macroscopic scale in standard polymer tests. However after several times recycling this will be a stronger effect. Maintaining the quality of recycled polymers over time hinges at the stabilisation of polymers at recycling. Stabilisation is realised through mixing in virgin polymers or additives at the compounding stage of recycling. Currently this in inherent to the recycling process, because a lot of plastic packaging material is made from virgin polymers.

Recyclability of plastics

As was described in Section 4.2 detergent bottles are highly suitable for applying large quantities of recycled polymers. In the transition to a circular economy bottle-to-bottle recycling is desirable: recycling polymers from used detergent bottles and using these for the production of new bottles[32]. This strategy is preferred over cascading the recycled polymers to other applications. The next paragraphs will evaluate the feasibility of bottle-to-bottle recycling for HDPE, PP and PET detergent bottles.

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Bottle-to-bottle recycling

HDPE flakes from detergent bottles are well recyclable. rHDPE typically has a low melt flow index (MFI) which makes it suitable for extrusion blow moulding (EBM) of new detergent bottles. This means that bottle-to-bottle recycling can be realised. In the market examples are seen in which high percentages of rHDPE (97%) are used in detergent bottles.

Application of rHDPE beyond EBM is limited because it cannot be applied in food applications[33] and is is generally unsuitable for injection blow moulding (IBM). This could be an argument to promote the uptake of rHDPE in detergent bottles, as it stimulates the demand.

PP flakes from detergent bottles are well recyclable. However, most PCR PP comes from injection moulded or thermoformed plastic packaging. Typically, these have a high MFI, opposed to the low

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[32] In practice, of course, recycling of detergent bottles is not a closed loop system. Detergent bottles are collected, sorted and recycled along with other plastic packaging waste. This means bottle-to-bottle recycling of detergent bottles also depends on the quality of other collected plastic packaging.
[33] Food application of rHDPE is possible when it can be proven that the origin of the recycled polymer is food grade. However, this requires a closed loop recycling system, which is not common practice.

MFI required for EBM. Therefore recycled PP is characterised by a high MFI. rPP with a low MFI is difficult to source, and therefore is not adopted by producers to make bottles using EBM. Consequently, the material loop of PP is difficult to close for the application in detergent bottles.

PET flakes from detergent bottles are well recyclable. However, application of PCR PET from these bottles is limited. Recycling of transparent PET is focussed on food grade quality, detergent bottles are not food grade and would thus contaminate this stream. The quality of the flakes allows the production of new bottles, but the recycling system does not facilitate this at the moment. When the HolyGrail project is more developed this is expected to improve.

Table 6-3: Overview of bottle-to-bottle recycling of plastics

	Recyclability	Used in the production of new detergent bottles	Other applications of recycled plastic
HDPE			
PP		Properties of rPP are not fit for EBM and thus bottle-to-bottle recycling cannot be achieved.	Injection blow moulding products
PET		This is technically possible, but not executed in practice. rPET for detergent bottles is generally sourced from a food grade stream.	Applied in strapping for e.g. pallets (cascading). rPET from detergent bottles cannot be used for food applications.

Polymer consideration
For detergent bottles there should be aimed to realise bottle-to-bottle recycling. Evaluate the recyclability of the selected polymer and if the recycled polymer can be used as a feedstock for the production of new detergent bottles.

Safety issues in plastic recycling

[This part will be further investigated and described]

- Formal vs informal recycling

6.4 MECHANICAL RECYCLING - RECYCLABILITY OF PIGMENTS

Pigments are used to give a specific colour to HDPE detergent bottles. Using pigments to colour PET bottles is discouraged, and thus not further considered. Pigments influence sorting of the bottle and recyclability of the polymer.

Affecting bottle sorting

As is elaborated in section 6.2, usage of the carbon black pigment inhibits recognition of the packaging material in the sorting process. This means that packaging containing carbon black is not sorted in a mono-material stream. Therefore, usage of the carbon black pigment is discouraged for detergent bottles. Alternative pigments are available to create dark colours whilst maintaining recognition by NIR scanners[34]. However, from a recycling perspective dark colours are not desirable in general, because these influence the colour of the whole rHDPE-stream (unless a colour sorter is present).

Dark pigments decrease value of recycling stream

In general a masterbatch contains 5-10% pigments. In a rHDPE bottle a masterbatch of about 3% is required. Thus the bottle consist for approximately for 0,15-0,3% out of pigments. This percentage is quite small and is regarded as a contamination in the recycling stream. The more pigments are added and the darker these are, the darker the recycled HDPE stream becomes. Dark coloured plastics are difficult to recolour with pigments and are thus of less value and in low demand by the market. As this effect is undesirable it is recommended to use light coloured pigments, prevent excessive use of pigments, and prevent dark pigments in detergent bottles. This promotes many reuse cycles of the polymer. This recommendation is not solely applicable for detergent bottles, but for all rigid HDPE packaging that ends up in the packaging waste stream.

Colour sorting: High-tech recycling facilities have colour sorters that sort can sort plastic flakes in different colours. Dark colours are separated from light colours and white flakes (containing titanium dioxide) are also sorted out. This enables a wider colour range for bottles made from recycled plastic, as lighter flakes are easier to recolour. This reduces the need for pigments in the masterbatch. However, colour sorters are not (yet) common practice in recycling facilities and should thus not be relied upon. Additionally, colour sorting does not improve the recyclability of dark coloured polymers, but merely makes them less disturbing (KIDV, 2019). In light of achieving the sustainable design goal *Closing material loops* it is thus recommended to only use light pigments.

Chemical consideration

When mechanical recycling is considered, the following rules need to be adhered to:

- Avoid carbon black as a pigment for dark bottles. Carbon black prevents sorting of detergent bottles for recycling. (HDPE bottles)
- Prefer light pigments over dark pigments to avoid a dark coloured recycling stream. (HDPE bottles)
- Use as few pigments as possible. For example by only using pigments in the outer layer in extrusion blow moulding. (HDPE bottles)

6.5 INCINERATION AND LANDFILLING

Incineration

This scenario is undesirable. Bottles are recyclable and incineration would waste the invested materials.

[This part will be further investigated and described]

Incineration of pigments

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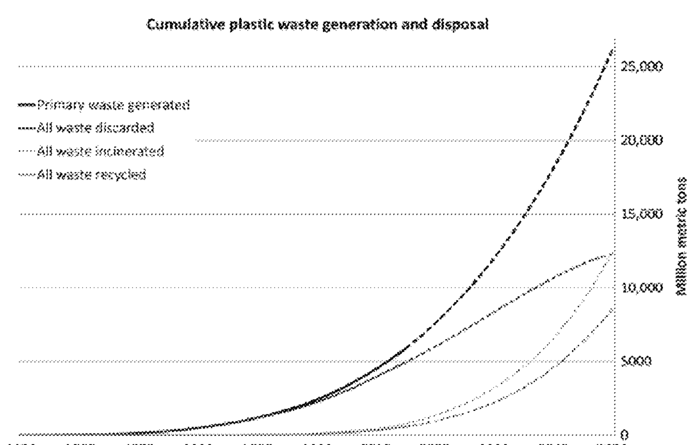
[34] Pigments 'Black 95491' and 'Black 95491' do not inhibit NIR detectability of the packaging (WRAP, 2011).

"Organic pigments completely degrade during combustion and the main oxidation products are usually carbon dioxide, water, and nitrogen. However, if a pigment contains other elements as well, further combustion products are formed. In particular, if a pigment contains halogens, small amounts of volatile organohalogen[35] compounds will be formed during combustion. These combustion products are likely to be persistent, bioaccumulative, and toxic. For these reasons, halogen-containing pigments should be excluded from use." (Cradle to Cradle Products Innovation Institute, 2019)

Landfilling of plastics

- "Around 6 300 million tonnes of plastics waste are thought to have been generated between 1950 and 2015, of which only 9% were recycled, and 12% incinerated, leaving nearly 80% to accumulate in landfills or the natural environment12. Plastic pollution is present in all the world's major ocean basins, including remote islands, the poles and the deep seas, and an additional 5 to 13 million tonnes are introduced every year13,14." (OECD, 2018)
- Capacity of landfills is finite: landfilling is not an activity that can be sustained over time. (Defra et al., 2006) [36]
- Landfills are leaking: to the soil, but also to marine environment
- Concerns around landfilling, further addressed in the next paragraphs:
    - Wildlife ingesting plastics or getting entangled in plastic waste
    - Creation of microplastics
    - Leakage of additive chemicals to the environment and transfer of these chemicals to animals and humans
- Because research on the effects of plastics in landfills, and the environment in general, is still relatively new there is still a lot of uncertainty. Especially the long term effects are difficult to gauge. However, there is a consensus that plastic in the environment has negative effects and must be avoided.



[35] Pigments containing a covalent fluoro-carbon, chloro-carbon, bromo-carbon or iodo-carbon bond.
[36] Defra, E., Wilson, S., & Hannan, M. (2006). Review of England's Waste Strategy, Environmental Report under the 'SEA'Directive. *London, UK: DEFRA. Review. Plastics, the environment and human health RC Thompson et al, 2165*, 790-794.

Unsafe landfills

- Physical problems for wildlife resulting from ingestion or entanglement in plastic

Microplastics

- Over time, plastic degrades and decomposes over hundreds or thousands of years fragmenting into microplastics and nanoplastics.
- Microplastics enter the food chain and pose risks for human health
  - E.g. through fish and shellfish [37]
  - Microplastics can also be absorbed by roots of crops[38]
  - Microplastics is found in tap water and bottled water[39]
  - Still a lot is unknown about effects of microplastics. Large quantities of plastics have only been present in the environment for a relatively short period of time. Difficult to gauge its consequences (OECD, 2018)
- Uncertainty still about the effects of nanoplastics.
- Oxo-(bio)degradable: "A further complication is that degradable, as opposed to biodegradable, polymers (also called 'oxo-biodegradable', 'oxy-degradable' or 'UV-degradable') can also be made from oil-based sources but as a consequence are not biopolymers. These degradable materials are typically polyethylene together with additives to accelerate the degradation. They are used in a range of applications and are designed to break down under UV exposure and/or dry heat and mechanical stress, leaving small particles of plastic. They do not degrade effectively in landfills and little is known about the timescale, extent or consequences of their degradation in natural environments (Barnes *et al.* 2009; Teuten *et al.* 2009). Degradable polymers could also compromise the quality of recycled plastics if they enter the recycling stream. As a consequence, use of degradable polymers is not advocated for primary retail packaging (WRAP 2009). "[40]

Leakage of additive chemicals to the environment

- End up in environment and groundwater: "Phthalates and BPA are detectable in aquatic environments, in dust and, because of their volatility, in air "(Rudel *et al.* 2001, 2003).
- Additives of particular concern are
  - phthalate plasticizers "Phthalates can leach out of products because they are not chemically bound to the plastic matrix, and they have attracted particular attention because of their high production volumes and wide usage (Wagner & Oehlmann 2009; Talsness *et al.* 2009)."
  - BPA: "There is evidence, however, that landfills can present a significant source of contaminants, such as BPA, to aquatic environments. Efficient treatment approaches are available and are in use in some countries (Teuten *et al.* 2009)."
  - brominated flame retardants

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[37] Thompson, R. (2015), "Microplastics in the Marine Environment: Sources, Consequences and Solutions", in Marine Anthropogenic Litter, Springer International Publishing, Cham, http://dx.doi.org/10.1007/978-3-319-16510-3_7. http://dx.doi.org/10.1021/acs.est.7b02219.
[38] https://phys.org/news/2020-07-crop-microplastics.html
[39] Kosuth, M. et al. (2018), SYNTHETIC POLYMER CONTAMINATION IN GLOBAL DRINKING WATER, https://orbmedia.org/stories/invisibles_final_report/multimedia.
[40] https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2873021/#RSTB20090053C40

- anti-microbial agents

- Pose a threat to animal health and human health [41]:
  - There is considerable concern about the adverse effects of these chemicals on wildlife and humans (Meeker *et al.* 2009; Oehlmann *et al.* 2009).[42]
  - Phthalates and BPA have been shown to affect reproduction in all studied animal groups, to impair development in crustaceans and amphibians and to induce genetic aberrations. Molluscs, crustaceans and amphibians appear to be especially sensitive to these compounds, and biological effects are observed at environmentally relevant exposures in the low ng l^{-1} to µg l^{-1} range. In contrast, most effects in fish (except for disturbance in spermatogenesis) occur at higher concentrations. Most plasticizers appear to act by interfering with the functioning of various hormone systems, but some phthalates have wider pathways of disruption. Effect concentrations of plasticizers in laboratory experiments coincide with measured environmental concentrations, and thus there is a very real potential for effects of these chemicals on some wildlife populations. The most striking gaps in our current knowledge on the impacts of plasticizers on wildlife are the lack of data for long-term exposures to environmentally relevant concentrations and their ecotoxicity when part of complex mixtures.

Design consideration

- Promote DfR to increase chances that packaging will end up in recycling stream. Landfilling of plastics is truly undesirable.

Polymer consideration

- Prevent use oxo-degradable plastics: degradability of these plastics is not achieved in the landfill environment. Also, these type of plastics have negative effects when ending up in the recycling stream.

Chemical consideration

- Prevent additives that can leak to the environment: phthalate plasticizers, BPA, brominated flame retardants, anti-microbial agents

[41] https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2873012/
[42] https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2873021/#RSTB20090053C21

7. HKEY CONSIDERATIONS AND TRADE-OFFS

7.1 KEY CONSIDERATIONS

Key considerations are the most important sustainability aspects to base a material selection on. For a detergent bottle, the following hotspots are identified per life cycle stage

Material sourcing

- Prefer recycled (secondary non-renewable) feedstock for the production of detergent bottles. This contributes to a closed material loop and reduces the environmental impact of the packaging.
- Quality of the recycled feedstock and the different approaches to upgrade the quality.
- Availability of high quality recycled feedstock in preferred colours.
- Using food grade recycled feedstock for a non-food application.
- The risk of hazardous substances caused by contamination of the recycled feedstock or by the production of virgin resin.

Production

- Feasibility of common bottle production methods using recycled feedstock.
- Volume of plastic required from different feedstocks to package 1L of detergent.
- Use of dark pigments that contaminate the recycling stream.
- Distance between the production facility where the bottles are blown and the location where the bottles are filled. Transportation of empty bottles can eliminate other sustainability benefits gained for a specific production method.

Use phase

- Space efficiency of the bottle design to reduce CO_2 impact caused by transport movements.
- Selecting a material that provides the required barrier properties and has a sufficient chemical resistance for packaging the detergent, without requiring additional additives or coatings.
- Migration of polymer and chemical additives into washing detergent, causing these to end up in the sewage system or come into contact with user's skin (highly diluted).

End of life

- Design of the bottle facilitates optimal sorting of the rigids plastic bottle in mono-streams.
- Select polymers with which bottle-to-bottle recycling can be realised.
- The health and environmental risk in waste management of the degradation or incineration of the material.
- Prevent use oxo-degradable plastics: degradability of these plastics is not achieved in the landfill environment. Also, these type of plastics have negative effects when ending up in the recycling stream.

7.2 TRADE-OFFS

The decisions or constraints in one step of the life cycle influence the possibilities in the other stages. The table below indicates how constraints set in the top row of the table influence the stages in the most left column.

Table 7-1: Dependencies between decisions and constraints in one life cycle stage to the other stages.

How → influences ↓	Sourcing	Production	Use	End of use
Sourcing		Required additives for production Required material properties	Safety requirements Required barrier properties Required chemical resistance	Recyclability of material Secondary feedstock
Production	Production methods suitable for processing polymer		Bottle design	Recyclable bottle design
Use		Usability of bottle		Collection at end of life
End of use	End of Use options of polymers and additives.	Sortability and recyclability	Collection of used bottles	

Trade offs that need to be made concern reduction of material use through primary feedstock versus closing material loops through secondary feedstock. Outcomes of trade-offs depend on local situations.

Reduce material use	*vs*	*Close material loops*
Light weighting of the bottle to reduce material required might require polymers of virgin quality	Or	To effectively close material loops recycled content in bottles must be maximised, possibly leading to heavier designs
Reduce material use	*vs*	*Close material loops*
PET bottles requires less material in production compared to HDPE bottles		Recycled PET is sourced from a (scarce) food grade stream
Preserve natural capital	*vs*	*Close material loops*
Highly concentrated detergent leads to fewer transport movements but requires bottle with premium chemical resistance unavailable form recycled feedstock.	Or	Using recycled feedstock for bottling less concentrated detergent requiring more transport movements.
Prevent product spoilage	*vs*	*Close material loops*

Using additives and coatings to enhance product shelf life and strength of packaging.	Or	Recyclability of plastic bottle.

Trade-offs beyond sustainability

In the development of bottles sustainability is not the only topic on which trade-offs are made. Often sustainability of a bottle (design) is in conflict with the desired aesthetics for marketing purposes, or is driven by costs. Below a few of these trade-offs are highlighted.

Product marketing Transparent bottles have a sleek design, but require use of a UV barrier.	*vs*	*Close material loops* UV barriers compromise closing the material loop.
Product marketing Attractive qualities of virgin feedstock.	*vs* Or	*Preserve natural capital & close loops* Secondary feedstock with limited aesthetics but reduced environment footprint.
Cost reduction Low prices of virgin PET with premium aesthetics.	*vs* Or	*Close material loops* High prices for recycled feedstock with reduced aesthetics.

8. MATERIAL ASSESSMENT

In this chapter all material options are considered based on the sustainability criteria that emerged from the life cycle analysis. For material assessment the hybrid decision making method is applied. First, the polymers are assessed in Section 8.1, leading to a polymer shortlist. Subsequently, the chemical considerations are addressed in Section 8.2. Finally, Section 8.3 explores the considerations to be made in terms of design.

8.1 POLYMER SHORTLIST

First selection

Three types of polymer feedstock are available: primary fossil based, renewable, secondary. Based on Chapter 4 from a sustainability perspective this feedstock is prioritized as follows:

1. Secondary feedstock – recycled
2. Renewable feedstock
3. Primary fossil based feedstock

The required barrier properties and chemical resistance of a detergent bottle can be fulfilled using recycled plastics (secondary feedstock). Therefore use of primary fossil feedstock is discouraged, to enable closing the material loop and realise bottle-to-bottle recycling for detergent bottles. In the transition to a circular economy same-value recycling is essential. Virgin plastics can be used in the masterbatch or to upgrade the quality of the recycled polymer, but for this purpose use of renewable feedstock should be considered first.

The shortlisted polymers will first be assessed on the availability of renewable or secondary feedstock, renewability of the material itself and potential for bottle-to-bottle recycling. Based Table 8-1 it can be concluded that PP is not a sustainable polymer to apply in detergent bottle packaging. Recycled PP is not suitable for the production of bottles and renewable feedstock is not available. Therefore, PP will not be further considered as a polymer suitable for application in detergent bottles.

Table 8-1

	HDPE	PP	PET
Recycled feedstock available			
Recycled feedstock can be used for bottle production			
Plastic is recyclable			
Bottle-to-bottle recycling			
Renewable feedstock available			
Conclusion	Further investigated	Not further investigated	Further investigated

Polymer assessment

The second sequential selection is done through evaluating other sustainability criteria for the more detailed polymers. For both polymer types HDPE and PET, virgin and recycled feedstocks are considered. It is assumed that polymers from a biobased feedstock have the same characteristics as virgin feedstock.

Based on Table 8-2 a choice can be made between HDPE and PET. The polymers differ primarily in aesthetics (transparency) and chemical resistance. From a sustainability point of view recycled HDPE is the preferred feedstock for detergent bottles. The predominant concern for adoption of recycled PET is that it is primarily sourced from a food grade feedstock.***Please provide feedback on this statement, is this something you agree with?***

Table 8-2

	HDPE	rHDPE	PET	rPET
UV barrier				
Moisture barrier				
Gas barrier				
Transparency				
Resistance to surfactants				
Resistance to solvents*		**		
Resistance to caustics*		**		
Resistance to acids*		**		
Handle in design				
Can be used in the production of new bottles				
Conclusion		Preferred material		

** Not relevant for laundry detergents*

*** Is expected to be similar to virgin HDPE, but requires validation*

8.2 CHEMICAL CONSIDERATIONS

When a polymer is selected, the relevant chemical considerations need to be revisited to make decisions in the production process and for a safe and sustainable chemical selection. During the analysis of the life cycle, the following considerations have been encountered.

Barrier properties

- When using additives or coatings, carefully consider how these behave in the bottle. If not embedded in the polymer matrix it can potentially migrate into the detergent.
- A UV barrier can improve the shelf life of a detergent. A UV barrier can be provided by adding pigments to detergent bottles. This prevents usage of light stabiliser additives or UV barrier coatings.

Production of plastic and bottles

- Chemicals additives are added to the plastic to serve specific purposes but can have consequences for the sustainability of the plastic product. They might hamper recyclability or pose a toxicity risk to human health or biodiversity at any point in the lifecycle. It should be considered whether the addition of the chemicals to the plastic is indispensable or whether more sustainable alternatives can be chosen.
- Prefer organic pigments over inorganic pigments.
- Most pigments do not have health consequences because they are embedded in the polymer matrix and therefore exposure is limited.
- Avoid using halogen-containing pigments because the combustion products at incineration are toxic. Pigments containing a covalent fluoro-carbon, chloro-carbon, bromo-carbon or iodo-carbon bond should be avoided.
- Pigments containing toxic elements such as lead, cadmium, mercury, vanadium, chromium(VI), cobalt, nickel, arsenic, antimony or selenium should be avoided.
- Azo pigment containing one or more carcinogenic aromatic amines as defined in European regulation 76/769/EEC should be avoided.
- *[Will be further complimented based on the final research]*

End of use

- It is recommended to avoid using colour additives in PET as this compromises the recyclability of the material.
- **Pigments:** Avoid using carbon black as a pigment, because it prevents corrects sorting of detergent bottles and thus inhibits recycling
- **Pigments:** Prefer light pigments over dark pigments to avoid a dark coloured recycling stream. (HDPE bottles)
- **Pigments:** Use as few pigments as possible. For example by only using pigments in the outer layer in extrusion blow moulding. (HDPE bottles)
- **HDPE and PP:** Ensure the density of HDPE and PP used in bottles is not above 1g/cm3. Otherwise the plastic will not be sorted for recycling. Thus, use a mono-material and avoid fillers.
- When using additives or coatings on the bottle it is important to carefully consider if leakage can take place and end up in the detergent. If additives are not embedded in the polymer matrix migration can take place. If this scenario is likely, safety of the used additives or coating is essential. Consult REACH and RSL.
- **Additives:** Prevent additives that can leak to the environment: phthalate plasticizers, BPA, brominated flame retardants, anti-microbial agents

Guidelines to safe selection of chemical additives

For a safe chemical selection the next steps will need to be taken:

1. Check, in collaboration with your material supplier if necessary, whether the found chemical considerations involve any of the substances on the Restricted Substances List (RSL) of the Cradle to Cradle Products Innovation Institute.
2. If substances on the RSL are part of a chemical consideration, try to find an alternative substance for the intended goal.

3. If no alternative is possible, verify that the concentration of the substance is below the limit set in the RSL.
4. If incorporation of substances on the RSL is inevitable for the product, verify through relevant migration tests that these substances do not pose a hazard in the bottle lifecycle.
5. If steps 3 or 4 cannot be passed, revisit the material choice matrix and select another material or material combination.

8.3 DESIGN CONSIDERATIONS

The design of the bottle is of great influence on its sustainability, achievement of the sustainable design goals and recovery of the invested materials. Therefore this section describes the main considerations to be made in regard to the bottle design.

Space efficient design

- Optimise bottle design for efficient transportation to reduce transport movements and thus preserve natural capital. This means excessive curves, headspace and 'shoulders' should be avoided. Additionally it is recommended to only use a handle for bottles larger than 2 litres.

Design for recycling

When a bottle is mechanically recycled, investigate the local sorting and recycling process. In general, when mechanical recycling is considered the following design rules need to be adhered to, to allow sorting of the plastics in a bottle in clean mono-streams:

- **Labels:** Avoid the use of full body sleeves and PVC labels.
- **Labels:** Select the material and size of the label to enable correct sorting of the detergent bottle.
- **Closures:** Avoid fillers in PP and HDPE closures that increase the density above 1g/cm3 to enable the closure material to be separated from the plastic bottle. Use of fillers in PP and PE can increase the density of the polymer, causing it to sink instead of float. The recycling process is based on the floating property of PP and PE.
- **Adhesives:** Select adhesives for the label that are soluble or releasable in the washing process.
- Apply a watermark to the label or bottle to allow sorting of the packaging as part of the HolyGrail project.

9. CONCLUSION

[Conclusion will be added in the final draft]

10. GLOSSARY

[Glossary will be added in the final draft]

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